Full wwPDB EM Validation Report ⓘ

May 8, 2025 – 01:55 PM EDT

PDB ID	:	8VLP / pdb_00008vlp
EMDB ID	:	EMD-43341
Title	:	Composite structure of human FASN with NADPH in State 3
Authors	:	Schultz, K.; Marmorstein, R.
Deposited on	:	2024-01-11
Resolution	:	3.20 Å(reported)
Based on initial model	:	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:

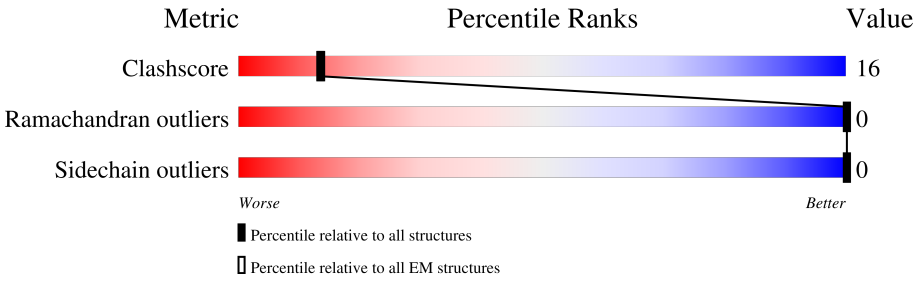
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	60% 21% 19%
1	B	2553	60% 21% 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 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
			25176	10041	9343	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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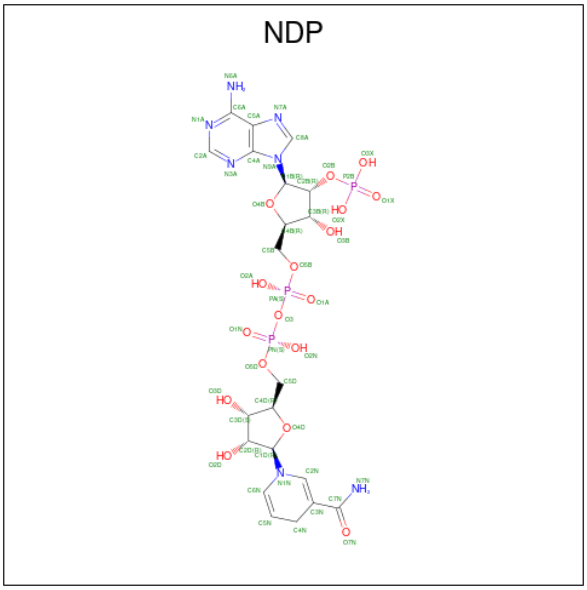
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
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).



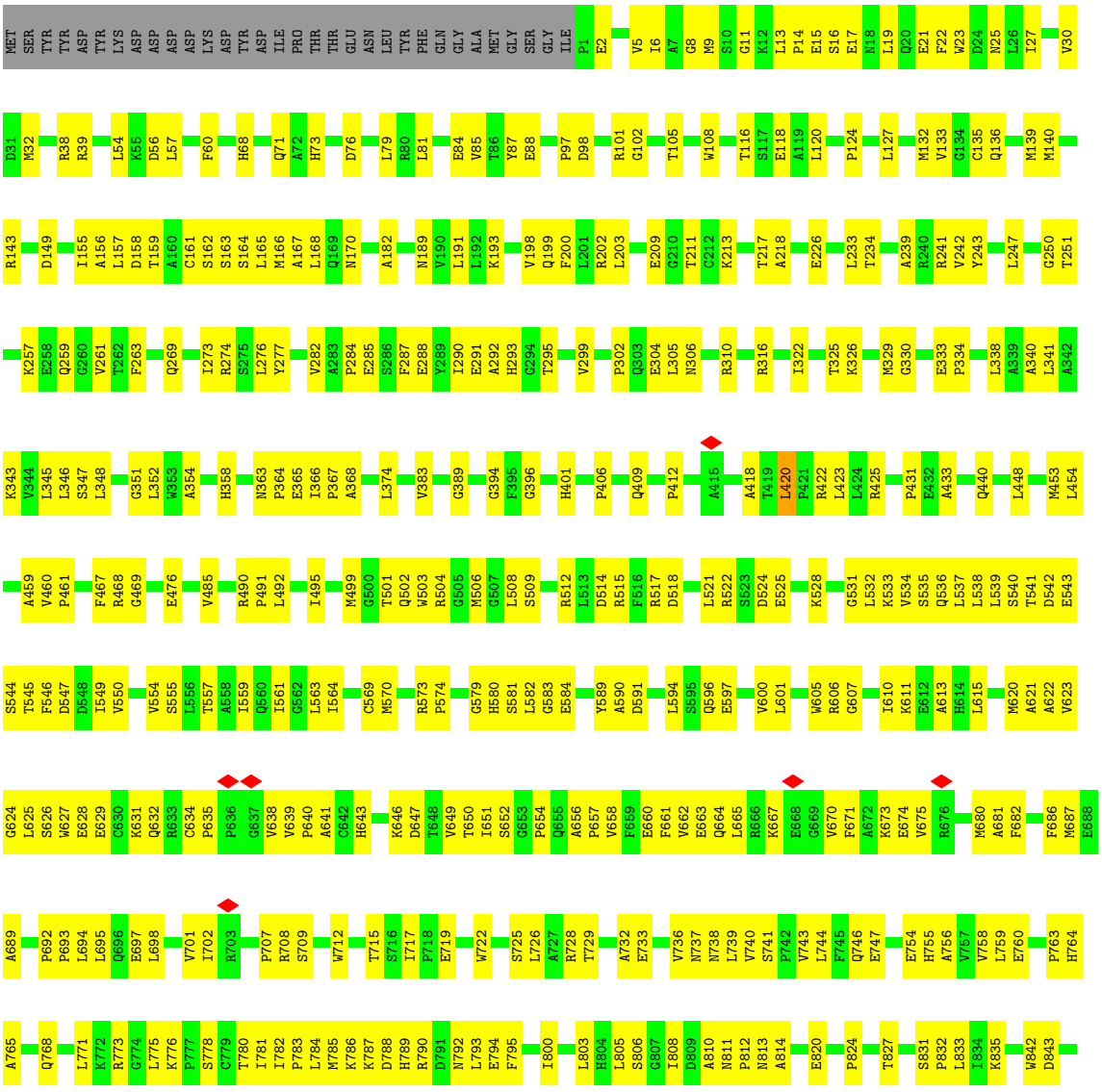
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

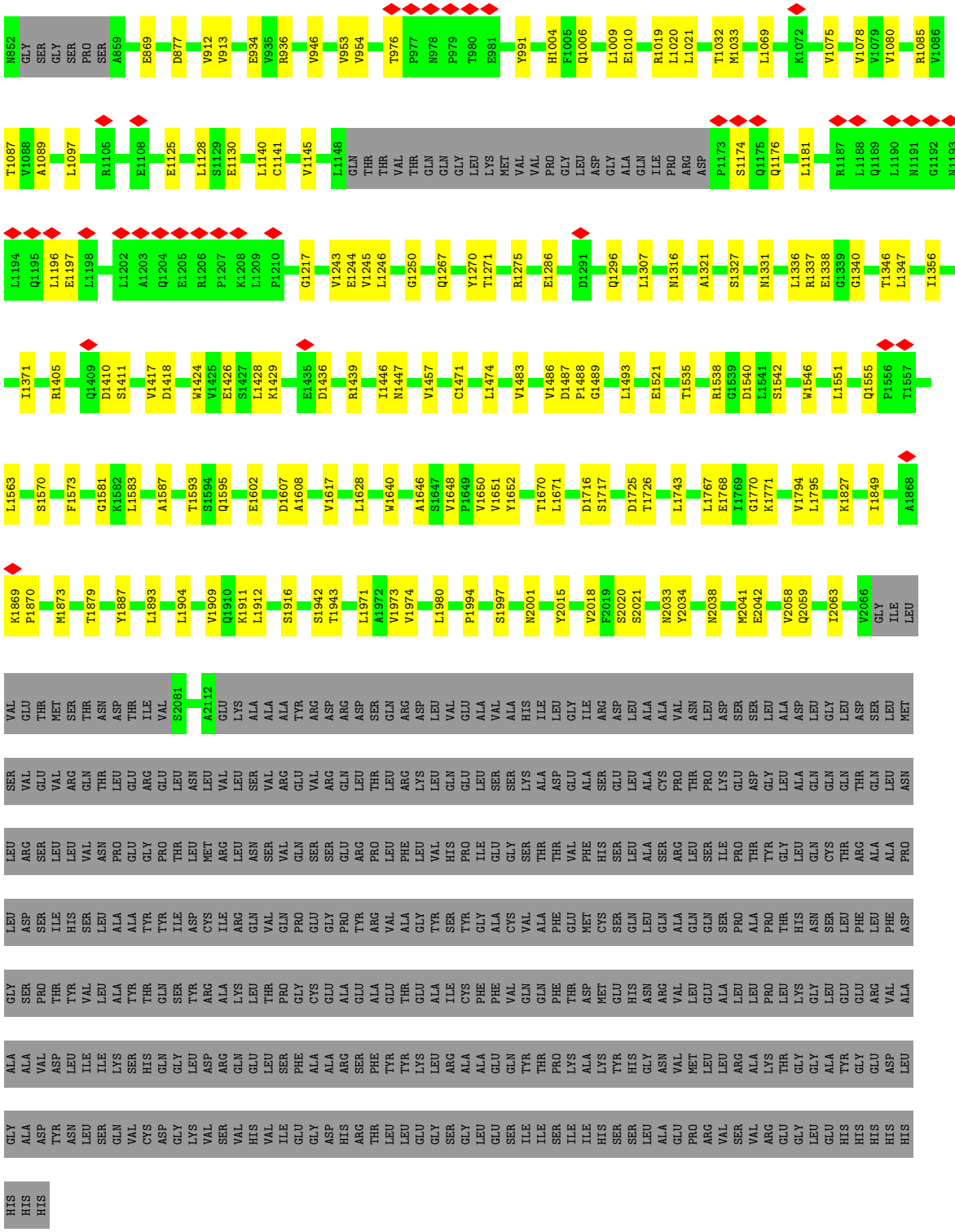
3 Residue-property plots (i)

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

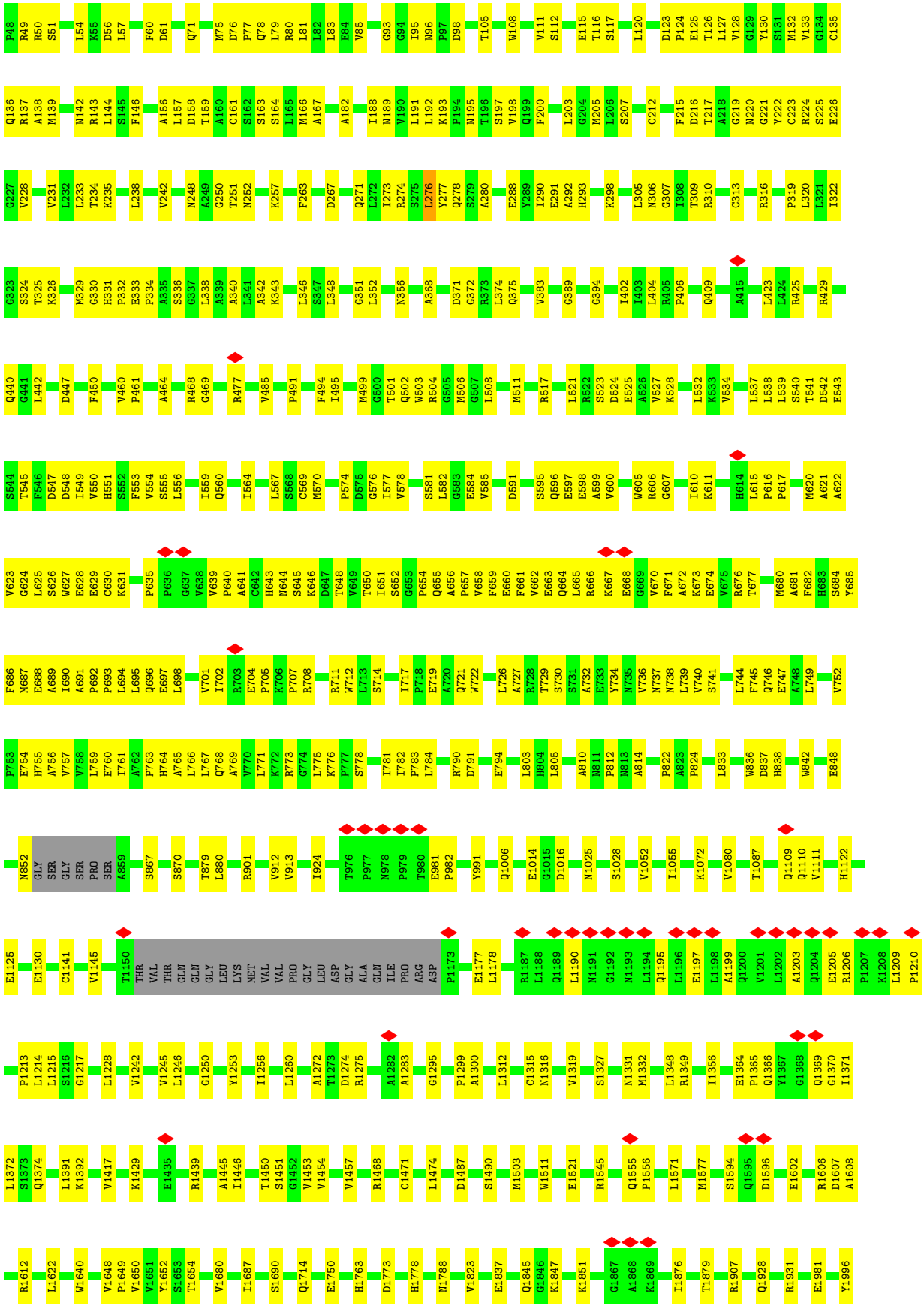
Chain A:

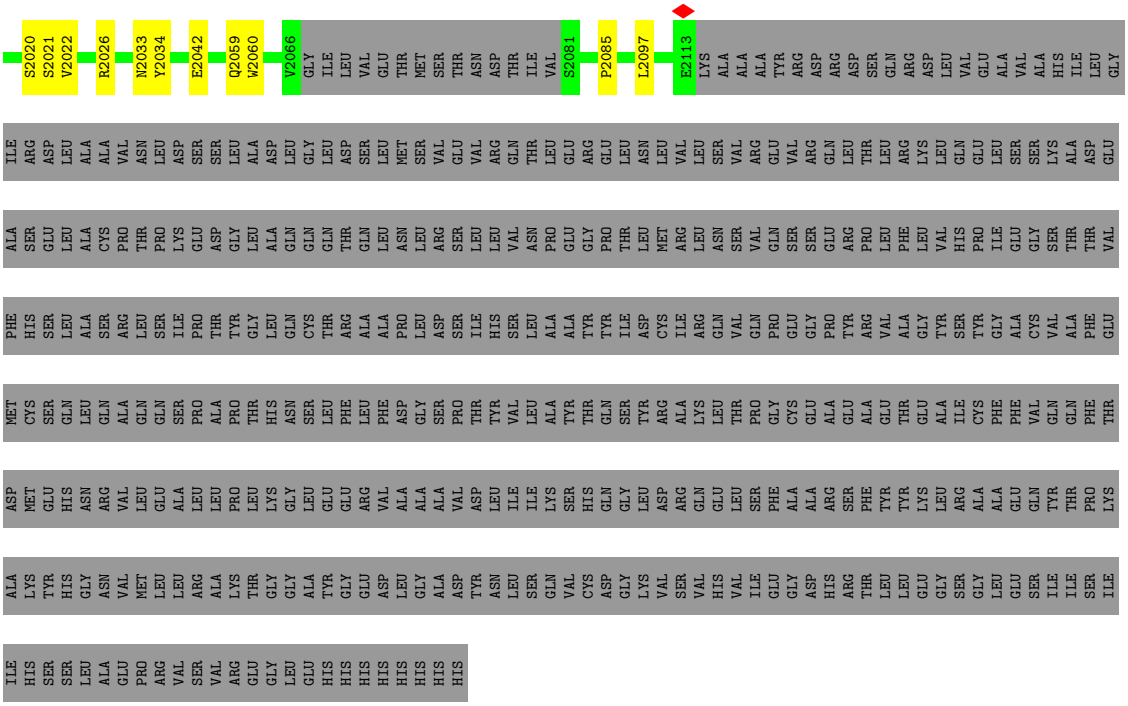




• Molecule 1: Fatty acid synthase

Chain B:


P48 R49 R50 S51 L54 K55 D56 L57 F60 D61 Q71 M75 D76 P77 Q78 L79 R80 L81 L82 L83 E84 V85 G93 G94 I95 N96 P97 D98 T105 W108 V111 S112 E115 T116 S117 L120 D123 P124 E125 T126 L127 V128 G129 Y130 S131 M132 V133 G134 C135
Q136 R137 A138 M139 N142 R143 L144 S145 F146 A156 L157 D158 T159 A160 C161 S162 S163 S164 L165 M166 A167 A182 I188 N189 V190 L191 L192 K193 P194 N195 T196 S197 V198 Q199 F200 L203 G204 M205 L206 S207 C212 F215 D216 T217 A218 G219 N220 G221 Y222 C223 R224 S225 E226
G227 V228 V231 L232 L233 T234 K235 L238 V242 N248 A249 G250 T251 N252 K257 F263 D267 Q271 L272 I273 R274 S275 L276 Y277 Q278 S279 A280 E288 Y289 I290 E291 A292 H293 K298 L305 N306 G307 I308 T309 R310 C313 R316 P319 L320 L321 I322
G323 S324 T325 K326 M329 G330 H331 P332 E333 P334 A335 S336 G337 L338 A339 A340 L341 A342 K343 L346 S347 L348 G351 L352 N356 A368 D371 G372 R373 L374 Q375 V383 G389 G394 I402 I403 L404 R405 P406 Q409 A415 L423 L424 R425 R429
Q440 G441 L442 D447 F450 V460 P461 A464 R468 G469 R477 V485 P491 F494 I495 M499 G500 T501 Q502 W503 R504 G505 M506 G507 L508 M511 R517 L521 R522 S523 D524 E525 A526 V527 K528 L532 K533 V534 L537 L538 L539 S540 T541 D542 E543
S544 T545 F546 D547 D548 I549 V550 H551 S552 F553 V554 S555 L556 I559 Q560 I564 L567 S568 C569 M570 P574 D575 G576 I577 V578 S581 L582 G583 E584 V585 D591 S595 Q596 E597 E598 A599 V600 W605 R606 G607 I610 K611 H614 L615 P616 P617 M620 A621 A622
V623 G624 L625 S626 W627 E628 E629 C630 K631 P635 P636 G637 V638 V639 P640 A641 C642 H643 N644 S645 K646 D647 T648 V649 T650 I651 S652 G653 P654 Q655 A656 P657 V658 F659 E660 F661 V662 E663 Q664 L665 R666 K667 E668 G669 V670 F671 A672 K673 E674 V675 R676 T677 M680 A681 F682 H683 S684 Y685
F686 M687 E688 A689 I690 A691 P692 P693 L694 L695 Q696 E697 L698 V701 I702 R703 E704 P705 K706 P707 R708 R711 W712 L713 S714 I717 P718 E719 A720 Q721 W722 L726 A727 R728 T729 S730 S731 A732 E733 Y734 N735 V736 N737 N738 L739 V740 S741 L744 F745 Q746 E747 A748 L749 V752
P753 E754 H755 A756 V757 V758 L759 E760 I761 A762 P763 H764 A765 L766 L767 Q768 A769 V770 L771 K772 R773 G774 L775 K776 P777 S778 I781 I782 P783 L784 R790 D791 E794 L803 H804 L805 A810 N811 P812 N813 A814 P822 A823 P824 L833 W836 D837 H838 W842 E848
N852 GLY SER GLY SER PRO SER A859 S867 S870 T879 L880 R901 V912 V913 I924 T976 P977 N978 P979 T980 E981 P982 Y991 Q1006 E1014 G1015 D1016 N1025 S1028 V1052 I1055 K1072 V1080 T1087 Q1109 Q1110 V1111 H1122
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 R1187 L1188 Q1189 L1190 N1191 G1192 N1193 L1194 Q1195 L1196 E1197 L1198 A1199 Q1200 V1201 L1202 A1203 Q1204 E1205 R1206 P1207 K1208 L1209 P1210
P1213 L1214 L1215 S1216 G1217 L1228 V1242 V1245 L1246 G1250 Y1253 I1256 L1260 A1272 T1273 D1274 R1275 A1282 A1283 G1295 P1299 A1300 L1312 C1315 N1316 V1319 S1327 N1331 M1332 L1348 R1349 I1356 E1364 P1365 Q1366 Y1367 G1368 Q1369 G1370 I1371
L1372 S1373 Q1374 L1391 K1392 V1417 K1429 E1435 R1439 A1445 I1446 T1450 S1451 G1452 V1453 V1454 V1457 R1468 C1471 L1474 D1487 S1490 M1503 W1511 E1521 R1545 Q1555 P1556 L1571 M1577 S1594 Q1595 D1596 E1602 R1606 D1607 A1608
R1612 L1622 W1640 V1648 P1649 V1650 V1651 Y1652 S1653 T1654 V1680 I1687 S1690 Q1714 E1750 H1763 D1773 H1778 N1788 V1823 E1837 Q1845 G1846 K1847 K1851 G1867 A1868 K1869 I1876 T1879 R1907 Q1928 R1931 E1981 Y1996


S2020 S2021 V2022 R2026 N2033 Y2034 E2042 Q2059 W2060 V2066 S2081 P2085 L2097 E2113

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131766	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	0.757	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.197	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	0.16	0/16198	0.26	1/22023 (0.0%)
1	B	0.20	0/16222	0.33	7/22055 (0.0%)
All	All	0.18	0/32420	0.30	8/44078 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	306	ASN	N-CA-C	-6.41	104.29	111.28
1	B	1649	PRO	N-CA-C	6.40	122.62	113.47
1	B	1649	PRO	CB-CA-C	-6.00	103.51	113.06
1	B	278	GLN	N-CA-CB	5.76	119.13	110.14
1	B	276	LEU	N-CA-C	5.64	117.12	110.97
1	B	278	GLN	N-CA-C	-5.61	102.97	111.56
1	B	1648	VAL	CB-CA-C	-5.42	108.61	114.35
1	A	420	LEU	N-CA-CB	5.31	117.86	110.11

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	9343	15809	517	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	15857	9380	15826	509	0
2	A	96	52	52	4	0
2	B	96	52	52	0	0
All	All	31882	18827	31739	1008	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 (1008) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLN:HA	1:A:506:MET:HE1	1.33	1.10
1:A:625:LEU:HD11	1:A:629:GLU:HB2	1.34	1.08
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.41	1.02
1:B:9:MET:HE1	1:B:342:ALA:HA	1.43	1.00
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.46	0.97
1:A:570:MET:HE3	1:A:810:ALA:HB1	1.47	0.94
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.53	0.92
1:B:687:MET:HA	1:B:690:ILE:HD13	1.52	0.92
1:B:626:SER:HB2	1:B:629:GLU:HG3	1.51	0.91
1:B:771:LEU:HB3	1:B:781:ILE:CD1	2.00	0.91
1:B:782:ILE:HG22	1:B:782:ILE:O	1.70	0.90
1:B:502:GLN:HG2	1:B:506:MET:HE1	1.52	0.90
1:A:440:GLN:HG3	1:A:833:LEU:HD22	1.51	0.89
1:A:13:LEU:HD22	1:A:329:MET:HE1	1.55	0.89
1:B:640:PRO:HA	1:B:651:ILE:HD13	1.55	0.89
1:B:654:PRO:HB2	1:B:657:PRO:HD2	1.53	0.88
1:A:164:SER:HB2	1:A:338:LEU:CD1	2.04	0.86
1:B:440:GLN:HG3	1:B:833:LEU:HD22	1.54	0.86
1:B:325:THR:HB	1:B:343:LYS:HD3	1.56	0.86
1:B:166:MET:HE1	1:B:251:THR:HG21	1.55	0.85
1:A:621:ALA:HA	1:A:674:GLU:HA	1.58	0.85
1:A:725:SER:HA	1:A:728:ARG:HH12	1.42	0.85
1:B:757:VAL:HG13	1:B:782:ILE:HD12	1.58	0.84
1:A:161:CYS:HB2	1:A:394:GLY:HA2	1.60	0.83
1:B:158:ASP:O	1:B:163:SER:HB3	1.77	0.83
1:A:22:PHE:HD1	1:A:32:MET:HE1	1.43	0.83
1:B:757:VAL:CG1	1:B:782:ILE:HD12	2.09	0.83
1:B:674:GLU:HG2	1:B:676:ARG:HH22	1.44	0.82
1:B:79:LEU:HD21	1:B:143:ARG:HG3	1.62	0.82
1:B:139:MET:HE3	1:B:139:MET:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.60	0.81
1:B:14:PRO:HD2	1:B:329:MET:HE2	1.63	0.81
1:B:752:VAL:O	1:B:776:LYS:NZ	2.13	0.81
1:A:420:LEU:HD21	1:A:512:ARG:HB3	1.63	0.81
1:B:623:VAL:HG12	1:B:625:LEU:HG	1.61	0.81
1:B:625:LEU:HD21	1:B:670:VAL:HG11	1.61	0.80
1:A:127:LEU:HD11	1:B:198:VAL:HG12	1.62	0.80
1:B:654:PRO:HB2	1:B:657:PRO:CD	2.11	0.80
1:B:682:PHE:HA	1:B:687:MET:SD	2.21	0.80
1:B:771:LEU:HB3	1:B:781:ILE:HD12	1.64	0.80
1:A:291:GLU:HG2	1:A:340:ALA:HB1	1.63	0.79
1:B:585:VAL:HG12	1:B:599:ALA:HB1	1.65	0.79
1:B:1773:ASP:OD1	1:B:1778:HIS:ND1	2.16	0.79
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.65	0.79
1:B:1837:GLU:N	1:B:1837:GLU:OE1	2.17	0.78
1:B:468:ARG:HD2	1:B:485:VAL:HG21	1.65	0.78
1:A:623:VAL:HG12	1:A:625:LEU:H	1.48	0.78
1:B:596:GLN:O	1:B:600:VAL:HG23	1.84	0.77
1:B:506:MET:HG3	1:B:559:ILE:HD11	1.66	0.77
1:A:656:ALA:HB3	1:A:657:PRO:HD3	1.67	0.77
1:A:418:ALA:HA	1:A:422:ARG:HH21	1.50	0.77
1:A:628:GLU:OE1	1:A:628:GLU:N	2.18	0.77
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.17	0.77
1:A:189:ASN:HD22	1:A:334:PRO:HD2	1.48	0.77
1:A:625:LEU:HD11	1:A:629:GLU:CB	2.15	0.77
1:A:468:ARG:HD2	1:A:485:VAL:HG21	1.66	0.77
1:A:365:GLU:N	1:A:365:GLU:OE1	2.17	0.76
1:B:771:LEU:HB3	1:B:781:ILE:HD11	1.66	0.76
1:B:623:VAL:HG21	1:B:665:LEU:HD13	1.67	0.76
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.67	0.76
1:A:570:MET:HE1	1:A:800:ILE:HD12	1.68	0.76
1:B:626:SER:HB2	1:B:629:GLU:CG	2.15	0.76
1:A:540:SER:HB3	1:A:545:THR:HG21	1.66	0.76
1:B:621:ALA:O	1:B:651:ILE:N	2.16	0.75
1:A:732:ALA:O	1:A:736:VAL:HG23	1.85	0.75
1:A:396:GLY:HA3	1:B:142:ASN:HD22	1.50	0.75
1:A:348:LEU:HD13	1:A:406:PRO:HB3	1.69	0.75
1:B:1109:GLN:N	1:B:1109:GLN:OE1	2.19	0.74
1:B:216:ASP:OD1	1:B:217:THR:N	2.20	0.74
1:B:182:ALA:CB	1:B:234:THR:HG22	2.17	0.74
1:A:687:MET:N	1:A:687:MET:HE2	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HB	1:B:242:VAL:HG13	1.69	0.74
1:B:511:MET:HE3	1:B:511:MET:O	1.88	0.74
1:A:725:SER:HA	1:A:728:ARG:NH1	2.02	0.74
1:B:540:SER:OG	1:B:545:THR:HG21	1.87	0.74
1:A:622:ALA:N	1:A:673:LYS:O	2.20	0.73
1:B:290:ILE:HG23	1:B:322:ILE:HD12	1.68	0.73
1:A:209:GLU:OE1	1:A:209:GLU:N	2.21	0.73
1:A:274:ARG:HA	1:A:277:TYR:CE2	2.22	0.73
1:A:694:LEU:O	1:A:698:LEU:HG	1.88	0.73
1:B:654:PRO:HG3	1:B:686:PHE:HZ	1.53	0.73
1:A:9:MET:HE1	1:A:345:LEU:HB3	1.68	0.73
1:B:164:SER:HB2	1:B:338:LEU:HG	1.70	0.73
1:B:757:VAL:HG13	1:B:782:ILE:CD1	2.18	0.73
1:A:596:GLN:O	1:A:600:VAL:HG23	1.90	0.72
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.70	0.72
1:A:506:MET:HG3	1:A:559:ILE:HD11	1.71	0.72
1:A:788:ASP:O	1:A:790:ARG:NH2	2.22	0.72
1:A:1010:GLU:OE2	1:A:1019:ARG:NH2	2.22	0.72
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.22	0.72
1:A:1716:ASP:OD1	1:A:1717:SER:N	2.22	0.72
1:B:620:MET:HE2	1:B:682:PHE:H	1.53	0.72
1:B:499:MET:HE1	1:B:581:SER:HB3	1.72	0.72
1:B:591:ASP:OD2	1:B:712:TRP:HB2	1.89	0.72
1:B:639:VAL:HG13	1:B:640:PRO:HD2	1.72	0.72
1:A:661:PHE:O	1:A:665:LEU:HG	1.90	0.71
1:B:663:GLU:O	1:B:667:LYS:HG3	1.90	0.71
1:A:657:PRO:O	1:A:660:GLU:HG2	1.89	0.71
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.23	0.71
1:A:200:PHE:CE2	1:B:132:MET:HE1	2.26	0.71
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.73	0.71
1:A:820:GLU:OE1	1:A:820:GLU:N	2.22	0.71
1:A:1337:ARG:NH1	1:A:1338:GLU:O	2.24	0.71
1:A:259:GLN:N	1:A:259:GLN:OE1	2.23	0.71
1:B:75:MET:HE3	1:B:79:LEU:HD23	1.72	0.71
1:B:672:ALA:O	1:B:673:LYS:HD2	1.91	0.71
1:A:737:ASN:OD1	1:A:741:SER:OG	2.08	0.70
1:B:719:GLU:HA	1:B:722:TRP:NE1	2.06	0.70
1:A:409:GLN:HB3	1:A:824:PRO:HA	1.74	0.70
1:A:79:LEU:HD21	1:A:143:ARG:HG3	1.72	0.70
1:B:694:LEU:HD23	1:B:698:LEU:HG	1.71	0.70
1:A:250:GLY:HA3	1:A:276:LEU:HD21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LEU:N	1:B:226:GLU:OE2	2.15	0.70
1:B:628:GLU:OE1	1:B:628:GLU:N	2.20	0.70
1:B:292:ALA:HB2	1:B:322:ILE:HD11	1.73	0.69
1:B:503:TRP:O	1:B:506:MET:HE3	1.92	0.69
1:B:622:ALA:HA	1:B:650:THR:HA	1.74	0.69
1:A:277:TYR:CE1	1:A:284:PRO:HG3	2.27	0.69
1:A:182:ALA:CB	1:A:234:THR:HG22	2.23	0.69
1:A:14:PRO:O	1:A:32:MET:HE2	1.92	0.69
1:A:293:HIS:N	1:A:304:GLU:OE2	2.23	0.69
1:A:502:GLN:HA	1:A:506:MET:CE	2.18	0.69
1:A:1426:GLU:OE1	1:A:1429:LYS:NZ	2.23	0.69
1:B:732:ALA:O	1:B:736:VAL:HG23	1.93	0.69
1:B:235:LYS:HE3	1:B:238:LEU:HD13	1.75	0.69
1:A:276:LEU:HD12	1:A:401:HIS:HB3	1.74	0.69
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.74	0.69
1:A:580:HIS:HD2	1:A:743:VAL:HG11	1.57	0.68
1:A:790:ARG:HA	1:A:790:ARG:NE	2.07	0.68
1:B:511:MET:HE1	1:B:517:ARG:HG3	1.75	0.68
1:A:646:LYS:HG3	1:A:647:ASP:OD1	1.92	0.68
1:B:708:ARG:NH2	1:B:714:SER:HB2	2.09	0.68
1:B:1206:ARG:NH2	1:B:1319:VAL:O	2.26	0.68
1:A:1033:MET:HE3	1:A:1089:ALA:HB3	1.76	0.68
1:A:1607:ASP:OD1	1:A:1608:ALA:N	2.27	0.68
1:A:549:ILE:HD11	1:A:611:LYS:HG3	1.75	0.68
1:A:584:GLU:HG3	1:A:712:TRP:HZ2	1.59	0.68
1:A:627:TRP:HA	1:A:649:VAL:HG21	1.76	0.68
1:B:429:ARG:NH1	1:B:464:ALA:O	2.26	0.68
1:B:503:TRP:H	1:B:506:MET:CE	2.06	0.68
1:A:628:GLU:HA	1:A:631:LYS:CE	2.21	0.67
1:A:620:MET:HE1	1:A:682:PHE:HB2	1.75	0.67
1:B:704:GLU:HG2	1:B:704:GLU:O	1.95	0.67
1:A:625:LEU:HD12	1:A:626:SER:H	1.58	0.67
1:B:60:PHE:CD1	1:B:80:ARG:HB3	2.29	0.67
1:A:503:TRP:CH2	1:A:506:MET:HA	2.29	0.67
1:B:549:ILE:HD11	1:B:553:PHE:CZ	2.30	0.67
1:A:22:PHE:CD1	1:A:32:MET:HE1	2.30	0.67
1:A:290:ILE:HG23	1:A:322:ILE:HG13	1.77	0.67
1:B:325:THR:HB	1:B:343:LYS:CD	2.25	0.67
1:B:719:GLU:HA	1:B:722:TRP:CE2	2.30	0.67
1:B:524:ASP:OD1	1:B:534:VAL:HB	1.95	0.67
1:B:697:GLU:O	1:B:701:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:O	1:B:138:ALA:HB2	1.95	0.66
1:B:112:SER:HB3	1:B:334:PRO:HG3	1.75	0.66
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.28	0.66
1:B:698:LEU:HB2	1:B:732:ALA:HB1	1.78	0.66
1:A:1275:ARG:O	1:A:1296:GLN:NE2	2.28	0.66
1:B:1228:LEU:HD21	1:B:1256:ILE:HD12	1.76	0.66
1:A:504:ARG:HA	1:A:546:PHE:CE1	2.30	0.66
1:A:1617:VAL:HG12	1:A:1628:LEU:HD13	1.76	0.66
1:B:504:ARG:HD2	1:B:543:GLU:OE1	1.95	0.66
1:A:663:GLU:O	1:A:667:LYS:HG2	1.95	0.66
1:A:57:LEU:HD23	1:A:81:LEU:HD11	1.78	0.66
1:A:768:GLN:HG3	1:A:781:ILE:HG21	1.77	0.66
1:B:215:PHE:CE1	1:B:305:LEU:HD11	2.31	0.66
1:B:685:TYR:HA	1:B:688:GLU:HG3	1.77	0.66
1:B:506:MET:HG3	1:B:559:ILE:CD1	2.26	0.66
1:B:757:VAL:CG1	1:B:782:ILE:CD1	2.73	0.66
1:A:506:MET:HG3	1:A:559:ILE:CD1	2.26	0.65
1:A:639:VAL:HB	1:A:640:PRO:HD2	1.77	0.65
1:B:782:ILE:O	1:B:782:ILE:CG2	2.43	0.65
1:B:1487:ASP:N	1:B:1490:SER:OG	2.30	0.65
1:A:1286:GLU:OE1	1:A:1286:GLU:N	2.29	0.65
1:A:84:GLU:O	1:A:88:GLU:HG3	1.96	0.65
1:A:440:GLN:HG3	1:A:833:LEU:CD2	2.23	0.65
1:A:640:PRO:HA	1:A:651:ILE:HG22	1.79	0.65
1:A:514:ASP:OD1	1:A:515:ARG:N	2.30	0.65
1:A:610:ILE:HG22	1:A:680:MET:HE1	1.79	0.65
1:B:447:ASP:OD2	1:B:450:PHE:HB2	1.96	0.65
1:B:537:LEU:HD11	1:B:551:HIS:ND1	2.12	0.65
1:B:1195:GLN:O	1:B:1199:ALA:N	2.29	0.65
1:A:694:LEU:O	1:A:694:LEU:HD12	1.98	0.65
1:B:182:ALA:HB2	1:B:234:THR:HG22	1.79	0.65
1:B:1327:SER:O	1:B:1331:ASN:ND2	2.29	0.64
1:A:21:GLU:O	1:A:25:ASN:ND2	2.30	0.64
1:A:189:ASN:ND2	1:A:333:GLU:OE1	2.28	0.64
1:A:625:LEU:CD1	1:A:629:GLU:HB2	2.22	0.64
1:B:620:MET:HE1	1:B:682:PHE:O	1.97	0.64
1:A:1997:SER:O	1:A:2001:ASN:ND2	2.30	0.64
1:B:620:MET:HG2	1:B:677:THR:HG21	1.79	0.64
1:A:161:CYS:HA	1:A:333:GLU:O	1.97	0.64
1:A:502:GLN:OE1	1:A:502:GLN:N	2.30	0.64
1:A:550:VAL:O	1:A:554:VAL:HG23	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:HD11	1:B:553:PHE:CE2	2.32	0.64
1:B:71:GLN:O	1:B:71:GLN:NE2	2.28	0.64
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.30	0.64
1:B:477:ARG:HH22	1:B:790:ARG:HD2	1.63	0.64
1:B:460:VAL:HG13	1:B:461:PRO:HD2	1.79	0.64
1:A:665:LEU:HB3	1:A:670:VAL:CG2	2.29	0.63
1:B:766:LEU:HD23	1:B:766:LEU:O	1.98	0.63
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.30	0.63
1:B:290:ILE:HG23	1:B:322:ILE:CD1	2.28	0.63
1:B:595:SER:N	1:B:598:GLU:OE1	2.19	0.63
1:B:501:THR:OG1	1:B:764:HIS:HB3	1.97	0.63
1:B:115:GLU:OE1	1:B:193:LYS:N	2.31	0.63
1:A:528:LYS:O	1:A:528:LYS:NZ	2.19	0.63
1:A:698:LEU:HB2	1:A:732:ALA:HB1	1.80	0.63
1:B:717:ILE:HD12	1:B:717:ILE:O	1.99	0.63
1:A:737:ASN:HA	1:A:740:VAL:HG22	1.81	0.63
1:B:662:VAL:O	1:B:666:ARG:HG2	1.98	0.63
1:B:659:PHE:O	1:B:663:GLU:HG3	1.98	0.63
1:A:274:ARG:HA	1:A:277:TYR:CD2	2.33	0.62
1:B:38:ARG:NH1	1:B:54:LEU:O	2.32	0.62
1:B:625:LEU:CD2	1:B:670:VAL:HG11	2.29	0.62
1:B:654:PRO:HG3	1:B:686:PHE:CZ	2.34	0.62
1:B:674:GLU:HG2	1:B:676:ARG:NH2	2.12	0.62
1:B:687:MET:HE3	1:B:739:LEU:HG	1.79	0.62
1:B:721:GLN:OE1	1:B:721:GLN:N	2.33	0.62
1:A:120:LEU:HD12	1:A:135:CYS:SG	2.40	0.62
1:A:627:TRP:CA	1:A:649:VAL:HG21	2.29	0.62
1:B:120:LEU:HD12	1:B:135:CYS:SG	2.40	0.62
1:B:687:MET:CE	1:B:739:LEU:HG	2.29	0.62
1:A:504:ARG:HA	1:A:546:PHE:HE1	1.62	0.62
1:B:139:MET:HE3	1:B:139:MET:CA	2.30	0.62
1:A:610:ILE:CG2	1:A:680:MET:HE1	2.30	0.62
1:A:627:TRP:CZ3	1:A:643:HIS:HB2	2.35	0.62
1:B:291:GLU:OE2	1:B:325:THR:HG22	1.99	0.62
1:B:567:LEU:HA	1:B:570:MET:CE	2.29	0.62
1:B:607:GLY:HA2	1:B:610:ILE:HD12	1.81	0.62
1:A:540:SER:CB	1:A:545:THR:HG21	2.30	0.61
1:A:692:PRO:O	1:A:695:LEU:HG	2.00	0.61
1:A:1942:SER:O	1:A:1943:THR:OG1	2.17	0.61
1:A:9:MET:HE3	1:A:243:TYR:CE1	2.35	0.61
1:A:247:LEU:HD23	1:A:282:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ARG:HH21	1:B:541:THR:HB	1.65	0.61
1:B:620:MET:HE2	1:B:682:PHE:N	2.14	0.61
1:B:1439:ARG:O	1:B:1468:ARG:NH1	2.34	0.61
1:A:211:THR:HG22	1:A:213:LYS:HG3	1.82	0.61
1:B:560:GLN:O	1:B:564:ILE:HG13	2.01	0.61
1:A:365:GLU:O	1:A:367:PRO:HD3	2.00	0.61
1:A:657:PRO:HA	1:A:660:GLU:HG2	1.82	0.61
1:B:469:GLY:HA2	1:B:805:LEU:HD21	1.82	0.61
1:A:431:PRO:HG3	1:A:467:PHE:CE2	2.36	0.61
1:B:111:VAL:HG13	1:B:137:ARG:HD2	1.82	0.61
1:A:628:GLU:CA	1:A:631:LYS:HE2	2.22	0.60
1:A:1893:LEU:HD12	1:A:1916:SER:OG	2.01	0.60
1:B:325:THR:HG21	1:B:340:ALA:HA	1.83	0.60
1:B:440:GLN:HG3	1:B:833:LEU:CD2	2.29	0.60
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.34	0.60
1:A:39:ARG:HD2	1:A:191:LEU:O	2.01	0.60
1:A:626:SER:HB3	1:A:629:GLU:CD	2.26	0.60
1:A:755:HIS:ND1	1:A:778:SER:HB2	2.16	0.60
1:B:189:ASN:HB2	1:B:334:PRO:HD2	1.82	0.60
1:B:767:LEU:O	1:B:771:LEU:HD23	2.01	0.60
1:B:664:GLN:HA	1:B:667:LYS:HD2	1.82	0.60
1:B:771:LEU:CB	1:B:781:ILE:HD12	2.32	0.60
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.33	0.60
1:A:495:ILE:HD12	1:A:771:LEU:HD21	1.84	0.60
1:A:629:GLU:OE1	1:A:629:GLU:N	2.27	0.60
1:A:831:SER:OG	1:A:832:PRO:HD3	2.01	0.60
1:B:166:MET:HE1	1:B:251:THR:CG2	2.29	0.60
1:B:736:VAL:O	1:B:740:VAL:HG22	2.01	0.60
1:B:1122:HIS:ND1	1:B:1511:TRP:O	2.34	0.60
1:A:418:ALA:HB2	1:A:448:LEU:HD11	1.83	0.60
1:B:1025:ASN:OD1	1:B:1028:SER:OG	2.15	0.60
1:B:705:PRO:HB3	1:B:730:SER:O	2.02	0.60
1:A:198:VAL:HG12	1:B:127:LEU:HD11	1.83	0.59
1:A:420:LEU:HD21	1:A:512:ARG:CB	2.30	0.59
1:A:518:ASP:O	1:A:522:ARG:HG3	2.02	0.59
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.33	0.59
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.34	0.59
1:A:200:PHE:CZ	1:B:132:MET:HE1	2.37	0.59
1:A:869:GLU:N	1:A:869:GLU:OE1	2.36	0.59
1:B:1205:GLU:O	1:B:1209:LEU:N	2.34	0.59
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:THR:HG22	1:A:364:PRO:HD3	1.84	0.59
1:A:506:MET:HE2	1:A:763:PRO:HB2	1.84	0.59
1:A:597:GLU:HG2	1:A:601:LEU:HD11	1.84	0.59
1:A:628:GLU:O	1:A:631:LYS:HG2	2.02	0.59
1:B:76:ASP:OD1	1:B:77:PRO:HD2	2.02	0.59
1:B:621:ALA:HA	1:B:674:GLU:HA	1.85	0.59
1:B:9:MET:CE	1:B:342:ALA:HA	2.26	0.59
1:B:548:ASP:HB3	1:B:551:HIS:HB2	1.85	0.59
1:A:508:LEU:HD11	1:A:538:LEU:O	2.03	0.59
1:B:182:ALA:HB1	1:B:234:THR:HG22	1.83	0.59
1:B:290:ILE:O	1:B:322:ILE:HD12	2.02	0.59
1:B:537:LEU:O	1:B:540:SER:OG	2.17	0.59
1:B:1250:GLY:O	1:B:1316:ASN:ND2	2.35	0.59
1:A:522:ARG:NH1	1:A:596:GLN:OE1	2.36	0.58
1:A:534:VAL:O	1:A:538:LEU:HG	2.03	0.58
1:B:291:GLU:HG2	1:B:340:ALA:HB1	1.85	0.58
1:B:501:THR:HG1	1:B:764:HIS:HB3	1.68	0.58
1:A:124:PRO:HG3	1:B:195:ASN:OD1	2.04	0.58
1:A:157:LEU:HD21	1:A:170:ASN:ND2	2.18	0.58
1:A:641:ALA:H	1:A:651:ILE:HA	1.68	0.58
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.86	0.58
1:B:664:GLN:OE1	1:B:667:LYS:HD2	2.04	0.58
1:A:503:TRP:H	1:A:506:MET:HE3	1.67	0.58
1:A:582:LEU:HD12	1:A:583:GLY:H	1.68	0.58
1:B:657:PRO:HA	1:B:660:GLU:OE1	2.03	0.58
1:A:654:PRO:HG3	1:A:686:PHE:HZ	1.69	0.58
1:A:6:ILE:HG12	1:A:233:LEU:HD21	1.86	0.58
1:A:159:THR:O	1:A:163:SER:HB3	2.04	0.58
1:A:561:ILE:HG23	1:A:589:TYR:CE2	2.38	0.58
1:A:629:GLU:CD	1:A:629:GLU:H	2.11	0.58
1:A:717:ILE:HG22	1:A:722:TRP:HD1	1.68	0.58
1:B:191:LEU:C	1:B:192:LEU:HD12	2.29	0.58
1:A:1551:LEU:HD12	1:A:1563:LEU:HD11	1.86	0.58
1:B:768:GLN:NE2	1:B:783:PRO:HB3	2.19	0.58
1:B:1300:ALA:O	1:B:1331:ASN:ND2	2.37	0.58
1:A:719:GLU:HA	1:A:722:TRP:CE2	2.39	0.58
1:A:514:ASP:OD1	1:A:515:ARG:HG2	2.04	0.58
1:B:273:ILE:O	1:B:277:TYR:CD2	2.56	0.58
1:B:274:ARG:HA	1:B:277:TYR:CE2	2.39	0.58
1:B:643:HIS:ND1	1:B:747:GLU:OE2	2.36	0.57
1:B:656:ALA:HB3	1:B:657:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ALA:CA	1:A:422:ARG:HH21	2.17	0.57
1:A:626:SER:HB3	1:A:629:GLU:OE2	2.03	0.57
1:B:623:VAL:CG1	1:B:625:LEU:HG	2.33	0.57
1:B:1199:ALA:O	1:B:1203:ALA:N	2.35	0.57
1:A:626:SER:HB3	1:A:629:GLU:OE1	2.03	0.57
1:A:719:GLU:HA	1:A:722:TRP:CD1	2.38	0.57
1:B:527:VAL:HG11	1:B:532:LEU:HD11	1.85	0.57
1:A:433:ALA:HB2	1:A:835:LYS:HB2	1.86	0.57
1:A:658:VAL:O	1:A:662:VAL:HG23	2.05	0.57
1:A:563:LEU:HD11	1:A:785:MET:HE3	1.86	0.57
1:A:733:GLU:OE1	1:A:733:GLU:N	2.27	0.57
1:A:737:ASN:HA	1:A:740:VAL:CG2	2.35	0.57
1:B:676:ARG:HG2	1:B:676:ARG:HH11	1.70	0.57
1:B:694:LEU:HD23	1:B:694:LEU:O	2.04	0.57
1:A:524:ASP:OD1	1:A:533:LYS:HA	2.04	0.57
1:B:622:ALA:N	1:B:673:LYS:O	2.23	0.57
1:B:673:LYS:HA	1:B:673:LYS:HE3	1.86	0.57
1:A:182:ALA:HB2	1:A:234:THR:HG22	1.86	0.57
1:A:460:VAL:HG13	1:A:461:PRO:HD2	1.87	0.57
1:B:11:GLY:HA2	1:B:85:VAL:CG1	2.34	0.57
1:B:161:CYS:HB2	1:B:394:GLY:HA2	1.86	0.57
1:B:623:VAL:CG2	1:B:665:LEU:HD13	2.35	0.57
1:B:692:PRO:O	1:B:696:GLN:HG3	2.04	0.57
1:A:182:ALA:HB1	1:A:234:THR:HG22	1.86	0.56
1:B:316:ARG:NH1	1:B:320:LEU:HB2	2.19	0.56
1:B:674:GLU:N	1:B:674:GLU:OE1	2.38	0.56
1:B:737:ASN:HA	1:B:740:VAL:CG2	2.34	0.56
1:B:1577:MET:N	1:B:1577:MET:HE2	2.20	0.56
1:A:341:LEU:O	1:A:345:LEU:HG	2.05	0.56
1:B:508:LEU:CD2	1:B:539:LEU:HD23	2.35	0.56
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.30	0.56
1:B:1928:GLN:OE1	1:B:1931:ARG:NH2	2.37	0.56
1:A:657:PRO:HA	1:A:660:GLU:CD	2.31	0.56
1:B:673:LYS:HA	1:B:673:LYS:CE	2.35	0.56
1:A:136:GLN:HB3	1:A:139:MET:HG2	1.87	0.56
1:A:13:LEU:HD13	1:A:329:MET:CE	2.34	0.56
1:B:761:ILE:HG12	1:B:784:LEU:HD11	1.88	0.56
1:A:524:ASP:HB2	1:A:534:VAL:HG22	1.87	0.56
1:B:105:THR:HG23	1:B:182:ALA:O	2.06	0.56
1:B:517:ARG:O	1:B:521:LEU:HG	2.06	0.56
1:B:136:GLN:HB3	1:B:139:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:LYS:H	1:A:776:LYS:HD2	1.71	0.56
1:B:771:LEU:O	1:B:775:LEU:HB2	2.04	0.56
1:A:635:PRO:HD3	1:A:661:PHE:CD1	2.41	0.56
1:A:503:TRP:HB3	1:A:787:LYS:HE3	1.88	0.55
1:A:780:THR:C	1:A:781:ILE:HD12	2.30	0.55
1:B:689:ALA:O	1:B:692:PRO:HD2	2.05	0.55
1:B:879:THR:C	1:B:880:LEU:HD12	2.32	0.55
1:A:9:MET:HE1	1:A:345:LEU:CB	2.36	0.55
1:A:1446:ILE:HG22	1:A:1474:LEU:HD12	1.88	0.55
1:B:225:SER:OG	1:B:330:GLY:HA3	2.06	0.55
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.06	0.55
1:A:412:PRO:HD3	1:A:824:PRO:HG2	1.88	0.55
1:B:508:LEU:HD21	1:B:539:LEU:HD23	1.88	0.55
1:B:576:GLY:C	1:B:577:ILE:HD12	2.31	0.55
1:B:719:GLU:HA	1:B:722:TRP:CD1	2.41	0.55
1:B:761:ILE:HA	1:B:784:LEU:HD12	1.87	0.55
1:A:8:GLY:HA2	1:A:243:TYR:HE2	1.71	0.55
1:A:299:VAL:O	1:A:302:PRO:HD2	2.07	0.55
1:B:22:PHE:CD1	1:B:32:MET:HE1	2.41	0.55
1:A:343:LYS:HE2	1:A:354:ALA:HB3	1.89	0.55
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.31	0.55
1:A:563:LEU:HD11	1:A:785:MET:CE	2.37	0.55
1:B:591:ASP:OD1	1:B:711:ARG:NH1	2.34	0.55
1:B:224:ARG:HG2	1:B:333:GLU:OE2	2.07	0.55
1:B:191:LEU:HG	1:B:226:GLU:CG	2.37	0.55
1:B:627:TRP:CZ3	1:B:640:PRO:HB2	2.42	0.55
1:B:769:ALA:O	1:B:773:ARG:HG2	2.07	0.55
1:A:1243:VAL:HG23	1:A:1271:THR:HG23	1.88	0.55
1:A:1250:GLY:O	1:A:1316:ASN:ND2	2.39	0.55
1:B:761:ILE:HG12	1:B:784:LEU:CD1	2.36	0.55
1:B:782:ILE:HG21	1:B:803:LEU:HD13	1.89	0.55
1:A:771:LEU:O	1:A:775:LEU:HB2	2.06	0.54
1:A:1428:LEU:HD22	1:A:1980:LEU:HD21	1.89	0.54
1:B:1445:ALA:O	1:B:1446:ILE:HD13	2.07	0.54
1:B:1545:ARG:HE	1:B:1876:ILE:HD11	1.70	0.54
1:A:976:THR:HG23	1:A:976:THR:O	2.07	0.54
1:B:656:ALA:O	1:B:660:GLU:HG3	2.07	0.54
1:A:351:GLY:C	1:A:352:LEU:HD12	2.33	0.54
1:B:157:LEU:O	1:B:157:LEU:HD12	2.06	0.54
1:A:420:LEU:HD11	1:A:512:ARG:HD2	1.89	0.54
1:A:652:SER:OG	1:A:681:ALA:HB1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HB3	1:B:372:GLY:O	2.07	0.54
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.41	0.54
1:A:293:HIS:CD2	1:A:295:THR:HG23	2.43	0.54
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.90	0.54
1:B:215:PHE:HE1	1:B:305:LEU:HD11	1.72	0.54
1:B:655:GLN:O	1:B:658:VAL:HG12	2.07	0.54
1:A:542:ASP:OD2	1:A:544:SER:OG	2.26	0.54
1:A:1446:ILE:HD12	1:A:1447:ASN:N	2.22	0.54
1:B:627:TRP:HB2	1:B:643:HIS:CD2	2.43	0.54
1:A:191:LEU:N	1:A:226:GLU:OE1	2.25	0.54
1:A:325:THR:HB	1:A:343:LYS:HD3	1.89	0.54
1:A:469:GLY:HA2	1:A:805:LEU:HD21	1.90	0.54
1:B:624:GLY:O	1:B:625:LEU:HD23	2.08	0.54
1:B:676:ARG:HA	1:B:676:ARG:NE	2.21	0.54
1:B:606:ARG:O	1:B:610:ILE:HG13	2.07	0.54
1:B:746:GLN:O	1:B:746:GLN:NE2	2.41	0.54
1:B:1228:LEU:HD21	1:B:1256:ILE:CD1	2.37	0.54
1:B:511:MET:HE1	1:B:517:ARG:CB	2.38	0.54
1:B:635:PRO:HD3	1:B:661:PHE:CE1	2.43	0.54
1:B:1879:THR:O	1:B:1907:ARG:NH1	2.41	0.54
1:A:333:GLU:HB2	1:A:334:PRO:CD	2.39	0.53
1:A:418:ALA:HA	1:A:422:ARG:NH2	2.20	0.53
1:B:402:ILE:HD12	1:B:404:LEU:HD21	1.90	0.53
1:B:537:LEU:HD11	1:B:551:HIS:CG	2.43	0.53
1:A:288:GLU:HG2	1:A:288:GLU:O	2.08	0.53
1:B:511:MET:HE1	1:B:517:ARG:HA	1.89	0.53
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.39	0.53
1:B:9:MET:HG3	1:B:19:LEU:CD1	2.37	0.53
1:B:790:ARG:HG3	1:B:791:ASP:N	2.24	0.53
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.90	0.53
1:A:557:THR:O	1:A:561:ILE:HG13	2.08	0.53
1:B:553:PHE:CD1	1:B:582:LEU:HD22	2.43	0.53
1:B:694:LEU:O	1:B:698:LEU:HG	2.08	0.53
1:A:647:ASP:OD2	1:A:773:ARG:HD3	2.09	0.53
1:B:205:MET:O	1:B:221:GLY:HA3	2.08	0.53
1:B:290:ILE:HD12	1:B:389:GLY:O	2.09	0.53
1:B:1272:ALA:O	1:B:1295:GLY:N	2.42	0.53
1:A:509:SER:HB2	1:A:792:ASN:HB2	1.90	0.53
1:A:661:PHE:CE2	1:A:665:LEU:HD21	2.44	0.53
1:B:348:LEU:HD13	1:B:406:PRO:HB3	1.91	0.53
1:B:511:MET:HE1	1:B:517:ARG:CG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:PRO:HG2	1:B:577:ILE:HD11	1.91	0.53
1:A:501:THR:OG1	1:A:763:PRO:HG2	2.09	0.53
1:B:534:VAL:O	1:B:538:LEU:HD13	2.09	0.53
1:B:1110:GLN:NE2	1:B:2085:PRO:O	2.41	0.53
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.89	0.53
1:B:235:LYS:HE3	1:B:238:LEU:CD1	2.38	0.53
1:A:660:GLU:HA	1:A:663:GLU:OE2	2.10	0.52
1:A:1794:VAL:O	1:A:1795:LEU:HD23	2.09	0.52
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.72	0.52
1:B:1555:GLN:N	1:B:1556:PRO:HD2	2.25	0.52
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.90	0.52
1:B:207:SER:HB2	1:B:220:ASN:HB2	1.91	0.52
1:A:760:GLU:OE2	1:A:765:ALA:HA	2.10	0.52
1:B:23:TRP:HB2	1:B:346:LEU:HD13	1.90	0.52
1:B:83:LEU:HD12	1:B:144:LEU:HD21	1.92	0.52
1:A:9:MET:HG3	1:A:19:LEU:CD1	2.40	0.52
1:A:76:ASP:HA	1:A:116:THR:HG21	1.91	0.52
1:A:504:ARG:HD2	1:A:541:THR:O	2.09	0.52
1:A:573:ARG:HD3	1:A:574:PRO:HD2	1.92	0.52
1:A:625:LEU:HD12	1:A:626:SER:N	2.23	0.52
1:B:504:ARG:HD2	1:B:543:GLU:CD	2.34	0.52
1:B:617:PRO:HB2	1:B:655:GLN:CD	2.35	0.52
1:B:1391:LEU:HD23	1:B:1392:LYS:N	2.25	0.52
1:B:371:ASP:OD1	1:B:372:GLY:N	2.37	0.52
1:A:698:LEU:O	1:A:702:ILE:N	2.23	0.52
1:A:597:GLU:CG	1:A:601:LEU:HD11	2.40	0.52
1:A:292:ALA:HB2	1:A:322:ILE:HD11	1.92	0.52
1:A:605:TRP:CD1	1:A:701:VAL:HG21	2.45	0.52
1:A:105:THR:HG23	1:A:182:ALA:C	2.34	0.52
1:B:1190:LEU:O	1:B:1195:GLN:NE2	2.42	0.52
1:B:1602:GLU:HB3	1:B:1650:VAL:HG23	1.92	0.52
1:A:68:HIS:HB3	1:A:71:GLN:OE1	2.10	0.52
1:A:261:VAL:HG12	1:B:146:PHE:CD1	2.45	0.52
1:A:623:VAL:HG12	1:A:625:LEU:N	2.22	0.52
1:B:754:GLU:OE2	1:B:778:SER:HB3	2.09	0.52
1:A:620:MET:HG2	1:A:652:SER:HB2	1.92	0.51
1:B:1080:VAL:HG22	1:B:1087:THR:HG23	1.92	0.51
1:A:1573:PHE:HE1	2:A:2601:NDP:H61A	1.58	0.51
1:B:324:SER:H	1:B:356:ASN:ND2	2.09	0.51
1:A:425:ARG:HD3	1:A:812:PRO:HD3	1.92	0.51
1:A:606:ARG:HH21	1:A:739:LEU:HD13	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1555:GLN:N	1:A:1555:GLN:OE1	2.42	0.51
1:A:476:GLU:N	1:A:794:GLU:OE2	2.37	0.51
1:B:1111:VAL:O	1:B:1111:VAL:HG13	2.10	0.51
1:A:1535:THR:HG23	1:A:1535:THR:O	2.10	0.51
1:B:1371:ILE:O	1:B:1372:LEU:HD12	2.10	0.51
1:A:1367:TYR:CE2	1:A:1371:ILE:HD11	2.46	0.51
1:B:159:THR:HG22	1:B:159:THR:O	2.10	0.51
1:B:495:ILE:CD1	1:B:578:VAL:HB	2.40	0.51
1:B:555:SER:O	1:B:559:ILE:HG13	2.11	0.51
1:A:202:ARG:NH1	1:B:127:LEU:O	2.43	0.51
1:A:580:HIS:CD2	1:A:743:VAL:HG11	2.42	0.51
1:A:786:LYS:HB3	1:A:789:HIS:HB2	1.93	0.51
1:B:737:ASN:HA	1:B:740:VAL:HG22	1.91	0.51
1:B:1471:CYS:SG	1:B:1503:MET:HE3	2.50	0.51
1:A:11:GLY:HA2	1:A:85:VAL:CG1	2.41	0.51
1:A:133:VAL:O	1:A:139:MET:HG3	2.11	0.51
1:A:1546:TRP:CD2	1:A:1873:MET:HE1	2.46	0.51
1:B:33:VAL:HB	1:B:50:ARG:NH2	2.25	0.51
1:B:550:VAL:O	1:B:554:VAL:HG23	2.10	0.51
1:B:658:VAL:O	1:B:662:VAL:HG23	2.11	0.51
1:B:60:PHE:HB3	1:B:842:TRP:CD1	2.46	0.50
1:B:491:PRO:HG2	1:B:756:ALA:HA	1.92	0.50
1:B:1016:ASP:O	1:B:1080:VAL:N	2.40	0.50
1:A:433:ALA:CB	1:A:835:LYS:HB2	2.42	0.50
1:A:694:LEU:HD12	1:A:698:LEU:HG	1.94	0.50
1:B:13:LEU:HD12	1:B:22:PHE:CG	2.46	0.50
1:B:203:LEU:HD13	1:B:205:MET:CE	2.41	0.50
1:B:708:ARG:HD2	1:B:734:TYR:CE2	2.46	0.50
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.11	0.50
1:A:579:GLY:O	1:A:715:THR:HG21	2.11	0.50
1:A:783:PRO:O	1:A:784:LEU:HB2	2.10	0.50
1:A:1457:VAL:HG11	1:A:1471:CYS:HB2	1.92	0.50
1:B:125:GLU:OE2	1:B:126:THR:N	2.44	0.50
1:B:687:MET:HE1	1:B:739:LEU:O	2.11	0.50
1:A:5:VAL:HB	1:A:242:VAL:HG13	1.94	0.50
1:A:9:MET:HE3	1:A:243:TYR:CD1	2.46	0.50
1:A:536:GLN:O	1:A:540:SER:OG	2.22	0.50
1:B:442:LEU:HD12	1:B:442:LEU:O	2.10	0.50
1:B:549:ILE:CG2	1:B:611:LYS:HG3	2.41	0.50
1:A:1128:LEU:HD21	1:A:1217:GLY:C	2.37	0.50
1:B:623:VAL:HG21	1:B:665:LEU:CD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MET:CE	1:A:345:LEU:CD1	2.90	0.50
1:A:168:LEU:HD23	1:A:168:LEU:O	2.12	0.50
1:A:364:PRO:HG2	1:A:365:GLU:OE1	2.11	0.50
1:A:1141:CYS:O	1:A:1145:VAL:HG23	2.11	0.50
1:B:191:LEU:O	1:B:192:LEU:HD12	2.10	0.50
1:A:584:GLU:HB2	1:A:738:ASN:HD21	1.76	0.50
1:A:692:PRO:HA	1:A:695:LEU:CD2	2.42	0.50
1:A:717:ILE:HD11	1:A:726:LEU:HB3	1.94	0.50
1:A:719:GLU:HA	1:A:722:TRP:NE1	2.27	0.50
1:B:625:LEU:HB2	1:B:630:CYS:SG	2.51	0.50
1:A:654:PRO:HB2	1:A:657:PRO:HD2	1.94	0.50
1:A:657:PRO:HA	1:A:660:GLU:CG	2.42	0.50
1:B:139:MET:HA	1:B:139:MET:CE	2.38	0.50
1:B:759:LEU:HD23	1:B:782:ILE:HG22	1.94	0.50
1:A:293:HIS:O	1:A:326:LYS:HD2	2.11	0.49
1:A:257:LYS:HE3	1:A:263:PHE:O	2.12	0.49
1:A:660:GLU:O	1:A:663:GLU:HG2	2.12	0.49
1:B:655:GLN:HA	1:B:658:VAL:HG12	1.93	0.49
1:B:1602:GLU:OE2	1:B:1851:LYS:NZ	2.45	0.49
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.45	0.49
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.45	0.49
1:B:617:PRO:HB2	1:B:655:GLN:OE1	2.11	0.49
1:A:217:THR:HG22	1:A:364:PRO:CD	2.43	0.49
1:A:396:GLY:HA3	1:B:142:ASN:ND2	2.25	0.49
1:A:641:ALA:N	1:A:650:THR:O	2.43	0.49
1:B:499:MET:HE1	1:B:581:SER:CB	2.39	0.49
1:B:1445:ALA:C	1:B:1446:ILE:HD13	2.37	0.49
1:A:276:LEU:CD1	1:A:401:HIS:HB3	2.42	0.49
1:A:635:PRO:HD3	1:A:661:PHE:CE1	2.48	0.49
1:A:746:GLN:O	1:A:746:GLN:NE2	2.46	0.49
1:B:51:SER:HA	1:B:223:CYS:SG	2.53	0.49
1:B:203:LEU:HD13	1:B:205:MET:HE3	1.93	0.49
1:B:685:TYR:HA	1:B:688:GLU:CG	2.42	0.49
1:A:1336:LEU:HD11	1:A:1340:GLY:HA3	1.95	0.49
1:A:1602:GLU:HB3	1:A:1650:VAL:HG23	1.95	0.49
1:B:521:LEU:O	1:B:525:GLU:HG2	2.12	0.49
1:A:25:ASN:HA	1:A:30:VAL:HG12	1.95	0.49
1:B:1014:GLU:OE1	1:B:1014:GLU:N	2.44	0.49
1:A:351:GLY:C	1:A:383:VAL:HG23	2.38	0.49
1:A:877:ASP:OD2	1:A:1004:HIS:ND1	2.46	0.49
1:B:191:LEU:HD22	1:B:224:ARG:NH2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:MET:HB2	1:B:682:PHE:CE2	2.47	0.49
1:B:1130:GLU:OE1	1:B:1130:GLU:N	2.40	0.49
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.43	0.49
1:A:299:VAL:C	1:A:302:PRO:HD2	2.38	0.49
1:A:412:PRO:HD3	1:A:824:PRO:CG	2.43	0.49
1:A:620:MET:HB2	1:A:675:VAL:CG1	2.43	0.49
1:B:1205:GLU:OE1	1:B:1209:LEU:HD12	2.13	0.49
1:A:620:MET:HE1	1:A:682:PHE:HD2	1.77	0.48
1:B:207:SER:HB3	1:B:221:GLY:N	2.28	0.48
1:B:623:VAL:HG13	1:B:671:PHE:O	2.13	0.48
1:B:645:SER:HB3	1:B:648:THR:OG1	2.13	0.48
1:B:692:PRO:HD2	1:B:693:PRO:HD2	1.94	0.48
1:B:745:PHE:CE2	1:B:749:LEU:HD11	2.48	0.48
1:A:673:LYS:HE3	1:A:674:GLU:O	2.12	0.48
1:A:783:PRO:HB2	1:A:795:PHE:HE2	1.78	0.48
1:A:1130:GLU:OE1	1:A:1130:GLU:N	2.42	0.48
1:A:1570:SER:OG	1:A:1646:ALA:O	2.22	0.48
1:B:691:ALA:O	1:B:695:LEU:N	2.33	0.48
1:B:701:VAL:HB	1:B:702:ILE:HD12	1.95	0.48
1:A:570:MET:HG2	1:A:811:ASN:O	2.13	0.48
1:A:692:PRO:HD2	1:A:693:PRO:HD2	1.95	0.48
1:A:694:LEU:HD11	1:A:698:LEU:HD11	1.94	0.48
1:A:1538:ARG:NH2	1:A:1581:GLY:O	2.46	0.48
1:B:584:GLU:HG3	1:B:738:ASN:OD1	2.13	0.48
1:A:953:VAL:HG22	1:A:954:VAL:HG23	1.95	0.48
1:A:1243:VAL:HG21	1:A:1307:LEU:HD13	1.94	0.48
1:B:123:ASP:HB3	1:B:126:THR:OG1	2.13	0.48
1:A:189:ASN:O	1:A:226:GLU:HB2	2.13	0.48
1:A:597:GLU:O	1:A:601:LEU:HG	2.14	0.48
1:B:643:HIS:ND1	1:B:746:GLN:HB3	2.28	0.48
1:A:535:SER:O	1:A:539:LEU:HD22	2.13	0.48
1:B:553:PHE:HE2	1:B:610:ILE:CD1	2.27	0.48
1:A:11:GLY:HA2	1:A:85:VAL:HG13	1.96	0.48
1:A:124:PRO:HA	1:A:127:LEU:CD2	2.44	0.48
1:A:161:CYS:CB	1:A:394:GLY:HA2	2.38	0.48
1:A:460:VAL:CG1	1:A:461:PRO:HD2	2.43	0.48
1:A:597:GLU:HG2	1:A:601:LEU:CD1	2.44	0.48
1:A:759:LEU:HD23	1:A:782:ILE:HB	1.94	0.48
1:B:547:ASP:OD1	1:B:548:ASP:N	2.46	0.48
1:B:768:GLN:NE2	1:B:781:ILE:HG21	2.29	0.48
1:A:189:ASN:HD22	1:A:334:PRO:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:LEU:O	1:A:670:VAL:HG22	2.14	0.48
1:A:1743:LEU:HD11	1:A:1767:LEU:HD11	1.96	0.48
1:B:124:PRO:HA	1:B:127:LEU:HD23	1.95	0.48
1:B:293:HIS:O	1:B:326:LYS:HD2	2.13	0.48
1:B:423:LEU:HD23	1:B:812:PRO:HB3	1.96	0.48
1:A:689:ALA:O	1:A:692:PRO:HD2	2.14	0.48
1:A:1909:VAL:HG11	1:A:1912:LEU:HD13	1.94	0.48
1:B:468:ARG:CD	1:B:485:VAL:HG21	2.39	0.48
1:A:302:PRO:HA	1:A:366:ILE:HD11	1.96	0.48
1:A:760:GLU:CD	1:A:765:ALA:HA	2.39	0.48
1:A:1196:LEU:HD12	1:A:1197:GLU:N	2.29	0.48
1:B:96:ASN:OD1	1:B:98:ASP:HB2	2.14	0.48
1:B:273:ILE:HG22	1:B:277:TYR:HE2	1.79	0.48
1:B:628:GLU:H	1:B:628:GLU:CD	2.16	0.48
1:A:627:TRP:CE3	1:A:643:HIS:HB2	2.49	0.47
1:A:2018:VAL:HG11	1:A:2041:MET:HB3	1.96	0.47
1:B:322:ILE:HG22	1:B:375:GLN:O	2.13	0.47
1:B:494:PHE:O	1:B:495:ILE:HD13	2.13	0.47
1:B:606:ARG:NH1	1:B:739:LEU:HB2	2.29	0.47
1:B:691:ALA:HB1	1:B:736:VAL:HG11	1.96	0.47
1:B:693:PRO:HA	1:B:696:GLN:OE1	2.14	0.47
1:A:199:GLN:HG2	1:B:127:LEU:HD13	1.95	0.47
1:A:542:ASP:O	1:A:545:THR:HG23	2.14	0.47
1:A:1418:ASP:OD2	1:A:1446:ILE:N	2.44	0.47
1:B:1750:GLU:N	1:B:1773:ASP:OD2	2.47	0.47
1:A:627:TRP:CZ3	1:A:640:PRO:HB2	2.50	0.47
1:A:1078:VAL:HA	1:A:1089:ALA:HB2	1.96	0.47
1:B:166:MET:CE	1:B:251:THR:HG21	2.35	0.47
1:B:191:LEU:HG	1:B:226:GLU:HG3	1.96	0.47
1:B:1612:ARG:NH2	1:B:1640:TRP:O	2.47	0.47
1:A:241:ARG:NH2	1:A:827:THR:O	2.47	0.47
1:A:1487:ASP:OD2	1:A:1489:GLY:N	2.45	0.47
1:B:56:ASP:OD1	1:B:57:LEU:N	2.48	0.47
1:B:212:CYS:SG	1:B:222:TYR:HA	2.55	0.47
1:B:1607:ASP:OD1	1:B:1608:ALA:N	2.46	0.47
1:A:56:ASP:OD1	1:A:57:LEU:N	2.48	0.47
1:A:490:ARG:HD3	1:A:806:SER:O	2.14	0.47
1:A:664:GLN:O	1:A:667:LYS:HB2	2.14	0.47
1:B:207:SER:HB3	1:B:221:GLY:O	2.14	0.47
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.38	0.47
1:B:585:VAL:HG12	1:B:599:ALA:CB	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:VAL:CG1	1:B:640:PRO:HD2	2.41	0.47
1:B:1366:GLN:O	1:B:1369:GLN:N	2.47	0.47
1:A:241:ARG:HD2	1:A:453:MET:CE	2.45	0.47
1:A:501:THR:HB	1:A:764:HIS:HB3	1.96	0.47
1:A:697:GLU:O	1:A:701:VAL:HG23	2.14	0.47
1:B:692:PRO:HB2	1:B:693:PRO:HD3	1.95	0.47
1:B:744:LEU:HB3	1:B:747:GLU:OE1	2.14	0.47
1:A:621:ALA:CA	1:A:674:GLU:HA	2.36	0.47
1:B:14:PRO:CD	1:B:329:MET:HE2	2.40	0.47
1:B:676:ARG:HG2	1:B:676:ARG:NH1	2.29	0.47
1:A:6:ILE:HG12	1:A:233:LEU:CD2	2.45	0.47
1:A:665:LEU:HB3	1:A:670:VAL:HG21	1.96	0.47
1:B:133:VAL:O	1:B:139:MET:HG3	2.14	0.47
1:B:409:GLN:OE1	1:B:409:GLN:HA	2.14	0.47
1:A:425:ARG:HH21	1:A:811:ASN:HD22	1.62	0.47
1:A:1794:VAL:C	1:A:1795:LEU:HD23	2.40	0.47
1:B:759:LEU:CD2	1:B:782:ILE:HG22	2.45	0.47
1:A:118:GLU:OE1	1:A:193:LYS:NZ	2.38	0.46
1:A:287:PHE:O	1:A:316:ARG:NH1	2.48	0.46
1:B:60:PHE:HB3	1:B:842:TRP:NE1	2.30	0.46
1:B:309:THR:O	1:B:313:CYS:HB2	2.15	0.46
1:B:543:GLU:OE1	1:B:543:GLU:HA	2.15	0.46
1:B:620:MET:CE	1:B:682:PHE:N	2.78	0.46
1:B:11:GLY:HA2	1:B:85:VAL:HG13	1.97	0.46
1:B:1652:TYR:CD1	1:B:1823:VAL:HG22	2.51	0.46
1:A:73:HIS:ND1	1:A:843:ASP:OD1	2.46	0.46
1:A:159:THR:HA	1:B:138:ALA:HB1	1.97	0.46
1:A:162:SER:OG	1:A:394:GLY:N	2.48	0.46
1:A:628:GLU:HG3	1:A:631:LYS:NZ	2.30	0.46
1:A:1346:THR:HG22	1:A:1347:LEU:N	2.30	0.46
1:B:425:ARG:NH1	1:B:810:ALA:O	2.48	0.46
1:B:511:MET:HE3	1:B:511:MET:CA	2.45	0.46
1:B:1206:ARG:CZ	1:B:1209:LEU:HD13	2.45	0.46
1:A:491:PRO:HG2	1:A:756:ALA:HA	1.97	0.46
1:A:717:ILE:HG22	1:A:722:TRP:CD1	2.50	0.46
1:B:523:SER:O	1:B:527:VAL:HG23	2.16	0.46
1:A:9:MET:CE	1:A:345:LEU:HD13	2.45	0.46
1:B:1246:LEU:HD11	1:B:1299:PRO:HG3	1.97	0.46
1:A:6:ILE:HA	1:A:233:LEU:HD23	1.98	0.46
1:A:108:TRP:HB3	1:A:167:ALA:HB1	1.98	0.46
1:B:33:VAL:CG1	1:B:50:ARG:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLN:HA	1:B:667:LYS:CD	2.45	0.46
1:B:745:PHE:O	1:B:749:LEU:HG	2.15	0.46
1:B:848:GLU:H	1:B:848:GLU:CD	2.23	0.46
1:A:425:ARG:HH22	1:A:459:ALA:HB2	1.80	0.46
1:A:549:ILE:HD11	1:A:607:GLY:O	2.15	0.46
1:A:569:CYS:SG	1:A:814:ALA:HB1	2.55	0.46
1:A:613:ALA:HB1	1:A:615:LEU:HG	1.97	0.46
1:B:502:GLN:HG2	1:B:506:MET:CE	2.37	0.46
1:A:728:ARG:HB2	1:A:728:ARG:CZ	2.46	0.46
1:B:606:ARG:NH1	1:B:739:LEU:HD13	2.31	0.46
1:B:620:MET:SD	1:B:652:SER:HB3	2.55	0.46
1:A:132:MET:HE3	1:B:200:PHE:CE1	2.51	0.46
1:A:694:LEU:HD12	1:A:694:LEU:C	2.40	0.46
1:B:11:GLY:HA2	1:B:85:VAL:HG11	1.97	0.46
1:B:13:LEU:HD22	1:B:329:MET:CE	2.46	0.46
1:B:22:PHE:CE1	1:B:32:MET:HE1	2.49	0.46
1:A:13:LEU:HD12	1:A:22:PHE:CG	2.51	0.46
1:A:155:ILE:HG22	1:A:156:ALA:N	2.31	0.46
1:A:1085:ARG:NH2	1:A:1097:LEU:O	2.49	0.46
1:B:9:MET:HG3	1:B:19:LEU:HD11	1.98	0.46
1:B:188:ILE:HG22	1:B:228:VAL:HG13	1.98	0.46
1:B:567:LEU:HA	1:B:570:MET:HE2	1.97	0.46
1:B:654:PRO:C	1:B:657:PRO:HD2	2.41	0.46
1:A:39:ARG:NH2	1:A:226:GLU:OE2	2.49	0.45
1:A:57:LEU:CD2	1:A:81:LEU:HD11	2.46	0.45
1:A:524:ASP:OD1	1:A:533:LYS:HG2	2.16	0.45
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.31	0.45
1:A:1768:GLU:OE2	1:A:1770:GLY:N	2.49	0.45
1:B:257:LYS:HE3	1:B:263:PHE:O	2.15	0.45
1:B:641:ALA:HB2	1:B:652:SER:HB3	1.98	0.45
1:B:791:ASP:OD2	1:B:794:GLU:HG3	2.16	0.45
1:A:213:LYS:HG2	1:A:358:HIS:HB3	1.98	0.45
1:A:506:MET:HE2	1:A:763:PRO:CB	2.46	0.45
1:A:627:TRP:HB2	1:A:643:HIS:CD2	2.51	0.45
1:A:657:PRO:C	1:A:660:GLU:HG2	2.41	0.45
1:B:668:GLU:HB2	1:B:670:VAL:HG23	1.99	0.45
1:A:347:SER:HB3	1:A:352:LEU:O	2.16	0.45
1:B:692:PRO:HB2	1:B:693:PRO:CD	2.45	0.45
1:A:707:PRO:HA	1:A:728:ARG:O	2.16	0.45
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.52	0.45
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:PRO:CG	1:B:577:ILE:HD11	2.46	0.45
1:B:1213:PRO:O	1:B:1217:GLY:N	2.50	0.45
1:A:13:LEU:HB3	1:A:14:PRO:CD	2.47	0.45
1:A:620:MET:HE1	1:A:682:PHE:CD2	2.52	0.45
1:A:638:VAL:HG11	1:A:651:ILE:HD12	1.97	0.45
1:B:112:SER:CB	1:B:334:PRO:HG3	2.45	0.45
1:B:597:GLU:CD	1:B:597:GLU:H	2.25	0.45
1:B:1315:CYS:SG	1:B:1332:MET:SD	3.15	0.45
1:A:531:GLY:C	1:A:532:LEU:HD22	2.42	0.45
1:A:573:ARG:HA	1:A:573:ARG:NE	2.32	0.45
1:A:692:PRO:HB2	1:A:693:PRO:HD3	1.98	0.45
1:A:503:TRP:CD1	1:A:787:LYS:HG3	2.52	0.45
1:B:203:LEU:CD1	1:B:205:MET:HE3	2.47	0.45
1:B:508:LEU:O	1:B:511:MET:HB2	2.17	0.45
1:B:534:VAL:CG2	1:B:554:VAL:HG12	2.47	0.45
1:B:620:MET:O	1:B:674:GLU:HA	2.17	0.45
1:B:677:THR:HB	1:B:682:PHE:HE2	1.81	0.45
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.52	0.45
1:B:1245:VAL:HB	1:B:1246:LEU:HD12	1.99	0.45
1:B:1451:SER:OG	1:B:1453:VAL:HG13	2.17	0.45
1:A:368:ALA:HB3	1:A:374:LEU:HD12	1.99	0.45
1:A:591:ASP:OD2	1:A:709:SER:HB3	2.16	0.45
1:A:5:VAL:HG21	1:A:239:ALA:HB2	1.97	0.45
1:A:5:VAL:HG21	1:A:239:ALA:CB	2.46	0.45
1:A:1971:LEU:N	1:A:1971:LEU:HD12	2.31	0.45
1:B:692:PRO:CD	1:B:693:PRO:HD2	2.47	0.45
1:A:15:GLU:OE2	1:A:38:ARG:NH2	2.49	0.45
1:A:420:LEU:HD23	1:A:793:LEU:CD2	2.47	0.45
1:B:499:MET:HA	1:B:556:LEU:CD2	2.47	0.45
1:B:627:TRP:NE1	1:B:631:LYS:HE2	2.31	0.45
1:A:105:THR:HG23	1:A:182:ALA:O	2.17	0.44
1:A:764:HIS:CG	1:A:787:LYS:HB2	2.52	0.44
1:B:351:GLY:C	1:B:352:LEU:HD12	2.42	0.44
1:B:556:LEU:HD12	1:B:763:PRO:HG3	1.99	0.44
1:B:687:MET:O	1:B:690:ILE:HB	2.17	0.44
1:A:702:ILE:N	1:A:702:ILE:HD12	2.32	0.44
1:A:736:VAL:O	1:A:740:VAL:HG22	2.16	0.44
1:A:1009:LEU:HD21	1:A:1021:LEU:HD21	2.00	0.44
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.42	0.44
1:A:363:ASN:HB3	1:A:366:ILE:HD13	1.98	0.44
1:A:646:LYS:HG3	1:A:647:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PRO:HB2	1:A:693:PRO:CD	2.48	0.44
1:A:692:PRO:CD	1:A:693:PRO:HD2	2.47	0.44
1:A:1140:LEU:HD13	1:A:1174:SER:OG	2.18	0.44
1:B:47:LEU:HD22	1:B:197:SER:HB3	2.00	0.44
1:B:251:THR:HG22	1:B:252:ASN:N	2.32	0.44
1:B:644:ASN:HB2	1:B:648:THR:OG1	2.16	0.44
1:B:681:ALA:O	1:B:684:SER:OG	2.21	0.44
1:A:606:ARG:O	1:A:610:ILE:HG13	2.18	0.44
1:A:811:ASN:OD1	1:A:813:ASN:HB2	2.17	0.44
1:A:1540:ASP:OD1	1:A:1542:SER:N	2.44	0.44
1:B:75:MET:HE2	1:B:75:MET:HB3	1.80	0.44
1:B:128:VAL:HG21	1:B:130:TYR:CZ	2.53	0.44
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.80	0.44
1:A:584:GLU:CB	1:A:738:ASN:HD21	2.30	0.44
1:A:708:ARG:N	1:A:728:ARG:O	2.43	0.44
1:A:733:GLU:H	1:A:733:GLU:CD	2.18	0.44
1:B:760:GLU:HB3	1:B:783:PRO:HA	1.99	0.44
1:A:13:LEU:HB3	1:A:14:PRO:HD2	1.99	0.44
1:A:468:ARG:CD	1:A:485:VAL:HG21	2.41	0.44
1:A:537:LEU:HA	1:A:540:SER:OG	2.17	0.44
1:A:1033:MET:CE	1:A:1089:ALA:HB3	2.46	0.44
1:B:447:ASP:HB3	1:B:450:PHE:HB3	2.00	0.44
1:B:1072:LYS:HD2	1:B:1072:LYS:N	2.33	0.44
1:B:1178:LEU:HD21	1:B:1215:LEU:HD11	1.99	0.44
1:A:8:GLY:HA2	1:A:243:TYR:CE2	2.50	0.44
1:A:17:GLU:HA	1:A:17:GLU:OE1	2.18	0.44
1:A:305:LEU:HD23	1:A:366:ILE:HG21	2.00	0.44
1:A:476:GLU:HG3	1:A:794:GLU:OE2	2.17	0.44
1:A:631:LYS:HG3	1:A:632:GLN:OE1	2.18	0.44
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.50	0.44
1:B:351:GLY:C	1:B:383:VAL:HG23	2.43	0.44
1:A:1887:TYR:HD1	1:A:1909:VAL:HG13	1.82	0.44
1:B:527:VAL:HG12	1:B:527:VAL:O	2.17	0.44
1:B:620:MET:O	1:B:674:GLU:HB2	2.18	0.44
1:B:694:LEU:HD23	1:B:694:LEU:C	2.43	0.44
1:B:867:SER:O	1:B:870:SER:OG	2.36	0.44
1:B:1348:LEU:HD22	1:B:1374:GLN:HB3	1.99	0.44
1:A:934:GLU:OE1	1:A:936:ARG:NH2	2.51	0.43
1:A:1640:TRP:CZ3	1:A:1648:VAL:HG21	2.53	0.43
1:B:83:LEU:HD12	1:B:144:LEU:CD2	2.48	0.43
1:B:219:GLY:O	1:B:298:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG23	1:B:822:PRO:HB3	2.00	0.43
1:B:740:VAL:HG23	1:B:741:SER:H	1.83	0.43
1:B:836:TRP:HB2	1:B:838:HIS:NE2	2.33	0.43
1:B:1242:VAL:HA	1:B:1312:LEU:O	2.17	0.43
1:B:1714:GLN:OE1	1:B:1714:GLN:N	2.47	0.43
1:A:132:MET:HE1	1:B:200:PHE:CE2	2.53	0.43
1:A:2021:SER:HA	2:A:2602:NDP:H5N	2.00	0.43
1:B:1214:LEU:HD12	1:B:1214:LEU:C	2.43	0.43
1:B:2097:LEU:O	1:B:2097:LEU:HD23	2.17	0.43
1:A:158:ASP:HB2	1:B:156:ALA:O	2.18	0.43
1:A:532:LEU:HD22	1:A:532:LEU:N	2.33	0.43
1:A:790:ARG:HH11	1:A:790:ARG:HG2	1.82	0.43
1:A:1771:LYS:HE3	1:A:1795:LEU:HD22	2.00	0.43
1:B:81:LEU:O	1:B:85:VAL:HG23	2.18	0.43
1:B:332:PRO:O	1:B:336:SER:HB3	2.18	0.43
1:A:60:PHE:HB3	1:A:842:TRP:CD1	2.53	0.43
1:A:351:GLY:O	1:A:352:LEU:HD12	2.17	0.43
1:A:425:ARG:HD3	1:A:812:PRO:CD	2.48	0.43
1:A:503:TRP:CG	1:A:787:LYS:HG3	2.52	0.43
1:B:250:GLY:HA3	1:B:276:LEU:HD21	2.01	0.43
1:B:288:GLU:O	1:B:288:GLU:HG2	2.19	0.43
1:B:307:GLY:HA2	1:B:310:ARG:CZ	2.49	0.43
1:B:1607:ASP:CG	1:B:1608:ALA:N	2.77	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.83	0.43
1:A:544:SER:O	1:A:547:ASP:HB3	2.19	0.43
1:A:634:CYS:HB3	1:A:638:VAL:O	2.17	0.43
1:A:686:PHE:HB2	1:A:687:MET:CE	2.49	0.43
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	2.00	0.43
1:B:635:PRO:HD3	1:B:661:PHE:CD1	2.53	0.43
1:B:1364:GLU:N	1:B:1365:PRO:HD2	2.34	0.43
1:A:306:ASN:HB3	1:A:310:ARG:HH12	1.83	0.43
1:A:1827:LYS:NZ	1:A:1849:ILE:O	2.44	0.43
1:B:117:SER:HB3	1:B:135:CYS:HB3	2.01	0.43
1:B:542:ASP:HB3	1:B:545:THR:OG1	2.17	0.43
1:A:495:ILE:HD12	1:A:758:VAL:HG11	2.00	0.43
1:A:620:MET:HB2	1:A:675:VAL:HG13	2.01	0.43
1:A:1275:ARG:NH2	1:A:1321:ALA:O	2.52	0.43
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.18	0.43
1:B:768:GLN:HE22	1:B:781:ILE:CG2	2.32	0.43
1:A:261:VAL:HG12	1:B:146:PHE:CG	2.53	0.43
1:A:423:LEU:HD23	1:A:812:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ILE:HD12	1:A:550:VAL:N	2.34	0.43
1:B:1454:VAL:HG13	1:B:1503:MET:HE1	2.01	0.43
1:A:241:ARG:HD2	1:A:453:MET:HE1	2.00	0.43
1:A:499:MET:HE1	1:A:581:SER:OG	2.19	0.43
1:A:542:ASP:OD1	1:A:543:GLU:N	2.52	0.43
1:A:754:GLU:HG3	1:A:778:SER:OG	2.18	0.43
1:A:1080:VAL:HG22	1:A:1087:THR:HG23	2.00	0.43
1:B:54:LEU:HD12	1:B:57:LEU:HD21	2.00	0.43
1:B:93:GLY:O	1:B:95:ILE:HD12	2.19	0.43
1:B:726:LEU:HD23	1:B:726:LEU:C	2.43	0.43
1:B:745:PHE:CE2	1:B:749:LEU:HD21	2.54	0.43
1:A:425:ARG:HH21	1:A:811:ASN:ND2	2.16	0.43
1:A:431:PRO:HG3	1:A:467:PHE:CD2	2.54	0.43
1:A:502:GLN:HG3	1:A:546:PHE:HB3	2.01	0.43
1:A:763:PRO:O	1:A:785:MET:HG2	2.19	0.43
1:B:33:VAL:HG12	1:B:50:ARG:HB3	2.01	0.43
1:B:248:ASN:HB2	1:B:280:ALA:HB2	2.00	0.43
1:B:1845:GLN:OE1	1:B:1847:LYS:NZ	2.44	0.43
1:A:499:MET:HE3	1:A:499:MET:H	1.83	0.42
1:B:1349:ARG:HA	1:B:1371:ILE:HD11	2.01	0.42
1:A:584:GLU:CB	1:A:738:ASN:ND2	2.82	0.42
1:A:765:ALA:HB2	1:A:783:PRO:HB3	2.02	0.42
1:B:2:GLU:OE1	1:B:2:GLU:HA	2.19	0.42
1:B:6:ILE:HG23	1:B:231:VAL:CG1	2.49	0.42
1:B:76:ASP:HA	1:B:116:THR:HG21	2.00	0.42
1:B:368:ALA:HB1	1:B:374:LEU:HB2	2.01	0.42
1:A:168:LEU:HD23	1:A:168:LEU:C	2.45	0.42
1:A:492:LEU:HD11	1:A:759:LEU:CD1	2.49	0.42
1:A:784:LEU:HD23	1:A:784:LEU:HA	1.92	0.42
1:A:946:VAL:O	1:A:953:VAL:HG12	2.19	0.42
1:A:1879:THR:HG23	1:A:2015:TYR:OH	2.18	0.42
1:B:569:CYS:SG	1:B:814:ALA:HB1	2.59	0.42
1:B:584:GLU:HG3	1:B:738:ASN:CG	2.45	0.42
1:B:852:ASN:OD1	1:B:901:ARG:NH1	2.52	0.42
1:B:2022:VAL:HG13	1:B:2060:TRP:O	2.20	0.42
1:A:124:PRO:HG2	1:B:45:TYR:CZ	2.55	0.42
1:A:759:LEU:HD21	1:A:803:LEU:HD13	2.01	0.42
1:B:124:PRO:HA	1:B:127:LEU:CD2	2.50	0.42
1:A:517:ARG:O	1:A:521:LEU:HD23	2.19	0.42
1:A:555:SER:O	1:A:559:ILE:HG13	2.19	0.42
1:A:686:PHE:C	1:A:687:MET:HE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:LEU:O	1:A:1405:ARG:NE	2.53	0.42
1:B:79:LEU:O	1:B:83:LEU:HD13	2.19	0.42
1:B:646:LYS:HA	1:B:646:LYS:HD2	1.78	0.42
1:B:702:ILE:HD12	1:B:702:ILE:N	2.34	0.42
1:A:81:LEU:O	1:A:85:VAL:HG23	2.19	0.42
1:A:654:PRO:O	1:A:658:VAL:HG23	2.20	0.42
1:A:692:PRO:N	1:A:693:PRO:HD2	2.35	0.42
1:B:765:ALA:HB1	1:B:768:GLN:HE21	1.83	0.42
1:B:1253:TYR:OH	1:B:1283:ALA:HB1	2.19	0.42
1:A:776:LYS:HD2	1:A:776:LYS:N	2.34	0.42
1:A:1181:LEU:C	1:A:1181:LEU:HD23	2.44	0.42
1:A:2034:TYR:O	1:A:2038:ASN:ND2	2.47	0.42
1:B:231:VAL:HG12	1:B:233:LEU:HD12	2.00	0.42
1:A:155:ILE:N	1:A:155:ILE:HD12	2.34	0.42
1:A:290:ILE:HD12	1:A:389:GLY:O	2.19	0.42
1:A:418:ALA:N	1:A:422:ARG:HH21	2.18	0.42
1:A:707:PRO:HA	1:A:729:THR:HA	2.00	0.42
1:A:717:ILE:O	1:A:722:TRP:NE1	2.50	0.42
1:A:9:MET:CE	1:A:243:TYR:CD1	3.02	0.42
1:A:785:MET:HG3	1:A:792:ASN:OD1	2.19	0.42
1:B:123:ASP:CG	1:B:126:THR:HG23	2.45	0.42
1:B:127:LEU:HD12	1:B:127:LEU:C	2.45	0.42
1:B:326:LYS:NZ	1:B:336:SER:HB2	2.34	0.42
1:B:655:GLN:C	1:B:658:VAL:HG12	2.45	0.42
1:A:13:LEU:HB2	1:A:16:SER:OG	2.20	0.42
1:A:27:ILE:HD12	1:A:27:ILE:HA	1.88	0.42
1:A:166:MET:HE1	1:A:251:THR:OG1	2.20	0.42
1:B:35:ASP:OD1	1:B:49:ARG:HB3	2.20	0.42
1:B:61:ASP:OD2	1:B:837:ASP:HB3	2.20	0.42
1:B:504:ARG:HH21	1:B:541:THR:CB	2.31	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.93	0.41
1:A:624:GLY:N	1:A:671:PHE:O	2.38	0.41
1:A:1245:VAL:HG23	1:A:1246:LEU:HD12	2.01	0.41
1:B:409:GLN:HB3	1:B:824:PRO:HA	2.02	0.41
1:B:754:GLU:O	1:B:755:HIS:HB2	2.19	0.41
1:B:1521:GLU:N	1:B:1521:GLU:CD	2.78	0.41
1:B:1571:LEU:CD2	1:B:1622:LEU:HD11	2.49	0.41
1:A:1593:THR:HG22	1:A:1595:GLN:H	1.85	0.41
1:B:108:TRP:HB3	1:B:167:ALA:HB1	2.02	0.41
1:B:212:CYS:SG	1:B:223:CYS:N	2.89	0.41
1:B:698:LEU:HB2	1:B:732:ALA:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:LEU:HD11	1:A:1075:VAL:HG11	2.02	0.41
1:A:2020:SER:N	1:A:2058:VAL:O	2.47	0.41
1:A:79:LEU:HB2	1:A:140:MET:SD	2.61	0.41
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.93	0.41
1:A:1436:ASP:OD1	1:A:1436:ASP:N	2.52	0.41
1:A:2020:SER:OG	1:A:2021:SER:N	2.54	0.41
1:B:1246:LEU:HD12	1:B:1246:LEU:N	2.35	0.41
1:A:1244:GLU:OE1	1:A:1270:TYR:OH	2.39	0.41
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.20	0.41
1:A:2063:ILE:HG12	2:A:2602:NDP:C7N	2.50	0.41
1:B:664:GLN:O	1:B:667:LYS:HB2	2.20	0.41
1:B:326:LYS:HE3	1:B:331:HIS:CD2	2.55	0.41
1:B:687:MET:HE1	1:B:739:LEU:HG	2.02	0.41
1:B:1763:HIS:N	1:B:1788:ASN:O	2.53	0.41
1:A:54:LEU:HD12	1:A:57:LEU:HD21	2.01	0.41
1:A:79:LEU:CD2	1:A:143:ARG:HG3	2.46	0.41
1:A:127:LEU:C	1:A:127:LEU:HD12	2.46	0.41
1:A:285:GLU:H	1:A:285:GLU:CD	2.29	0.41
1:A:310:ARG:NH1	1:A:310:ARG:HG3	2.35	0.41
1:B:615:LEU:HB2	1:B:616:PRO:HD2	2.02	0.41
1:B:740:VAL:HG23	1:B:741:SER:N	2.36	0.41
1:B:981:GLU:N	1:B:982:PRO:HD3	2.35	0.41
1:B:1366:GLN:O	1:B:1370:GLY:N	2.52	0.41
1:B:1594:SER:OG	1:B:1596:ASP:OD1	2.39	0.41
1:A:269:GLN:O	1:A:273:ILE:HG13	2.20	0.41
1:A:754:GLU:O	1:A:755:HIS:HB2	2.21	0.41
1:A:1973:VAL:H	2:A:2602:NDP:H52A	1.84	0.41
1:B:654:PRO:HB2	1:B:657:PRO:CG	2.50	0.41
1:B:707:PRO:HA	1:B:729:THR:HA	2.02	0.41
1:B:726:LEU:HD23	1:B:727:ALA:N	2.35	0.41
1:B:1606:ARG:HE	1:B:1612:ARG:HG3	1.85	0.41
1:B:2020:SER:OG	1:B:2021:SER:N	2.52	0.41
1:A:23:TRP:HB2	1:A:346:LEU:HD13	2.03	0.41
1:A:87:TYR:CE1	1:A:97:PRO:HG2	2.55	0.41
1:A:348:LEU:HD13	1:A:406:PRO:CB	2.47	0.41
1:A:525:GLU:OE1	1:A:525:GLU:HA	2.20	0.41
1:A:620:MET:O	1:A:675:VAL:HG12	2.21	0.41
1:A:912:VAL:HG22	1:A:913:VAL:N	2.35	0.41
1:B:267:ASP:O	1:B:271:GLN:HG3	2.21	0.41
1:B:511:MET:HE1	1:B:517:ARG:CA	2.51	0.41
1:B:524:ASP:O	1:B:528:LYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LYS:HB3	1:B:528:LYS:HE2	1.87	0.41
1:B:1687:ILE:O	1:B:1690:SER:OG	2.38	0.41
1:A:492:LEU:HD13	1:A:808:ILE:CD1	2.51	0.41
1:A:641:ALA:HB2	1:A:652:SER:N	2.36	0.41
1:B:549:ILE:HG23	1:B:550:VAL:N	2.36	0.41
1:B:605:TRP:HD1	1:B:701:VAL:HG21	1.86	0.41
1:A:326:LYS:HA	1:A:330:GLY:O	2.21	0.40
1:A:606:ARG:NH2	1:A:739:LEU:HA	2.36	0.40
1:A:643:HIS:ND1	1:A:747:GLU:OE2	2.54	0.40
1:A:1869:LYS:NZ	1:A:1870:PRO:O	2.53	0.40
1:B:125:GLU:CD	1:B:125:GLU:C	2.89	0.40
1:B:1125:GLU:OE1	1:B:1125:GLU:N	2.54	0.40
1:A:98:ASP:HA	1:A:101:ARG:HG3	2.03	0.40
1:A:102:GLY:N	1:A:149:ASP:OD2	2.54	0.40
1:A:213:LYS:HE2	1:A:218:ALA:O	2.20	0.40
1:A:1521:GLU:OE1	1:A:1521:GLU:N	2.52	0.40
1:B:912:VAL:HG22	1:B:913:VAL:N	2.36	0.40
1:B:924:ILE:HD12	1:B:924:ILE:N	2.37	0.40
1:B:1052:VAL:HG11	1:B:1055:ILE:HD11	2.03	0.40
1:B:1450:THR:HG1	1:B:1996:TYR:HH	1.65	0.40
1:A:1583:LEU:HD11	1:A:1587:ALA:HB3	2.03	0.40
1:B:351:GLY:O	1:B:352:LEU:HD12	2.22	0.40
1:A:396:GLY:CA	1:B:142:ASN:HD22	2.25	0.40
1:B:685:TYR:CA	1:B:688:GLU:HG3	2.50	0.40
1:B:717:ILE:HD12	1:B:717:ILE:C	2.47	0.40
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.37	0.40
1:B:1228:LEU:HD23	1:B:1260:LEU:HD21	2.04	0.40
1:B:1654:THR:HG21	1:B:1680:VAL:HG22	2.04	0.40
1:B:2022:VAL:O	1:B:2026:ARG:N	2.52	0.40
1:A:2:GLU:OE1	1:A:2:GLU:HA	2.21	0.40
1:A:290:ILE:HG23	1:A:290:ILE:O	2.22	0.40
1:A:694:LEU:CD1	1:A:698:LEU:HD11	2.52	0.40
1:A:744:LEU:HB3	1:A:747:GLU:CG	2.51	0.40
1:A:1417:VAL:HG23	1:A:1424:TRP:CD2	2.57	0.40
1:B:2097:LEU:HD23	1:B:2097:LEU:C	2.45	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%)	2021 (98%)	39 (2%)	0	100	100
1	B	2063/2553 (81%)	2026 (98%)	37 (2%)	0	100	100
All	All	4123/5106 (81%)	4047 (98%)	76 (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%)	1705 (100%)	0	100	100
1	B	1708/2117 (81%)	1708 (100%)	0	100	100
All	All	3413/4234 (81%)	3413 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	A	306	ASN
1	A	331	HIS
1	A	580	HIS
1	A	644	ASN
1	A	852	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	863	ASN
1	A	971	HIS
1	A	1193	ASN
1	A	1504	ASN
1	A	1778	HIS
1	A	1792	HIS
1	A	2001	ASN
1	B	142	ASN
1	B	199	GLN
1	B	350	HIS
1	B	358	HIS
1	B	502	GLN
1	B	768	GLN
1	B	1278	GLN
1	B	1294	GLN
1	B	1331	ASN
1	B	1345	HIS
1	B	1447	ASN
1	B	1832	HIS
1	B	1848	HIS
1	B	2050	HIS
1	B	2100	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 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	-	47,52,52	0.68	0	61,80,80	0.77	2 (3%)
2	NDP	B	2602	-	47,52,52	0.65	0	61,80,80	0.88	3 (4%)
2	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.80	2 (3%)
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.87	2 (3%)

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	-	-	11/30/77/77	0/5/5/5
2	NDP	B	2602	-	-	10/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	8/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	12/30/77/77	0/5/5/5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2602	NDP	P2B-O2B-C2B	-3.97	112.82	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.90	113.01	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.81	107.36	109.92
2	B	2601	NDP	P2B-O2B-C2B	-2.66	116.32	123.43
2	B	2602	NDP	C3N-C2N-N1N	-2.57	119.44	123.20
2	B	2601	NDP	C5A-C6A-N6A	2.40	123.96	120.31
2	A	2602	NDP	C5A-C6A-N6A	2.29	123.80	120.31
2	A	2601	NDP	C5A-C6A-N6A	2.25	123.74	120.31
2	B	2602	NDP	C5A-C6A-N6A	2.09	123.50	120.31

There are no chirality outliers.

All (41) 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	C5B-O5B-PA-O2A
2	A	2602	NDP	C5B-O5B-PA-O3
2	A	2602	NDP	O4B-C4B-C5B-O5B
2	A	2602	NDP	C5D-O5D-PN-O3
2	A	2602	NDP	C5D-O5D-PN-O2N
2	B	2601	NDP	C5D-O5D-PN-O1N
2	B	2601	NDP	C2N-C3N-C7N-N7N
2	B	2602	NDP	C5B-O5B-PA-O1A
2	B	2602	NDP	C5B-O5B-PA-O2A
2	B	2602	NDP	O4D-C1D-N1N-C6N
2	B	2601	NDP	O4D-C1D-N1N-C2N
2	A	2602	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	O4B-C4B-C5B-O5B
2	B	2601	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	C3B-C2B-O2B-P2B
2	A	2602	NDP	O4D-C1D-N1N-C6N
2	A	2601	NDP	C1B-C2B-O2B-P2B
2	B	2602	NDP	C4B-C5B-O5B-PA
2	B	2602	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	O4D-C4D-C5D-O5D
2	A	2601	NDP	C2N-C3N-C7N-O7N
2	A	2601	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-O3
2	B	2602	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4B-C4B-C5B-O5B
2	B	2602	NDP	C4D-C5D-O5D-PN
2	B	2601	NDP	C3B-C2B-O2B-P2B
2	A	2601	NDP	C3B-C4B-C5B-O5B
2	A	2601	NDP	C2B-O2B-P2B-O1X
2	A	2602	NDP	C4B-C5B-O5B-PA
2	A	2601	NDP	C2B-O2B-P2B-O2X
2	B	2601	NDP	C2B-O2B-P2B-O3X
2	B	2602	NDP	C3B-C4B-C5B-O5B
2	B	2601	NDP	C1B-C2B-O2B-P2B
2	B	2601	NDP	PA-O3-PN-O1N

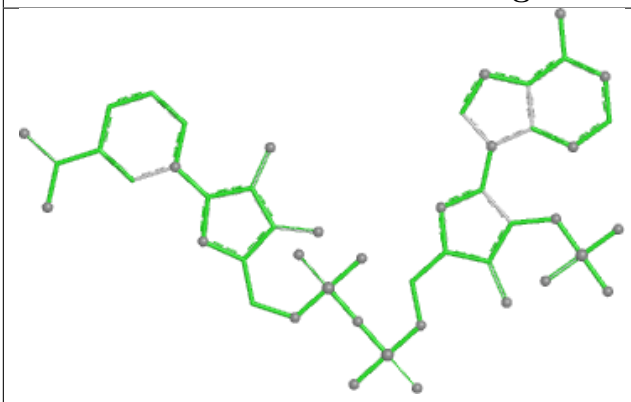
There are no ring outliers.

2 monomers are involved in 4 short contacts:

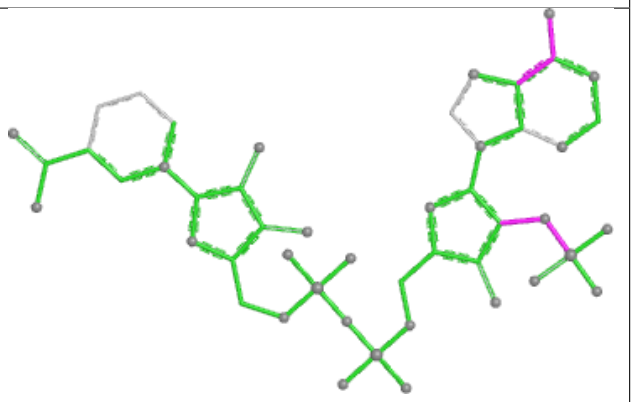
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2602	NDP	3	0
2	A	2601	NDP	1	0

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.

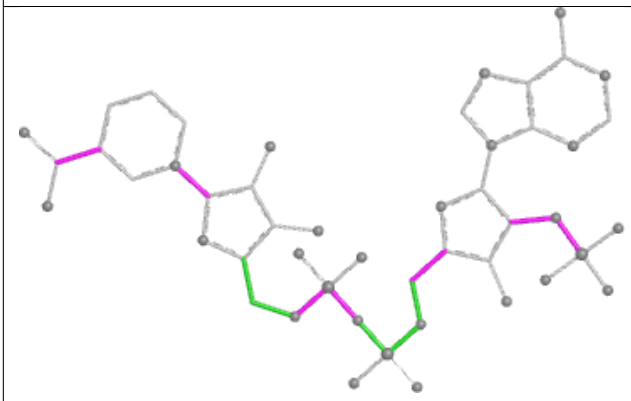
Ligand NDP B 2601



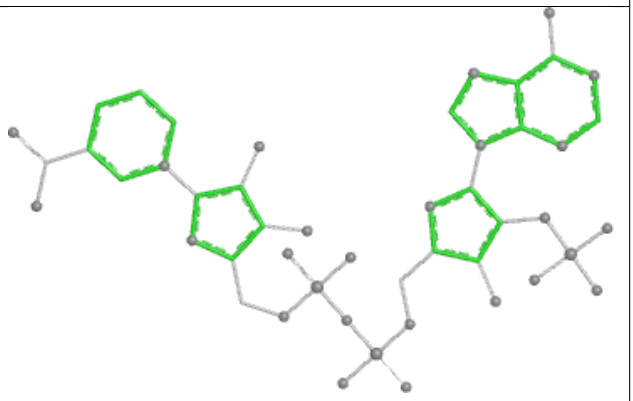
Bond lengths



Bond angles

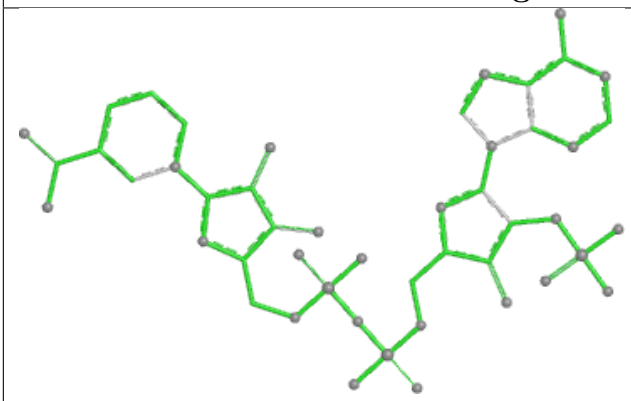


Torsions

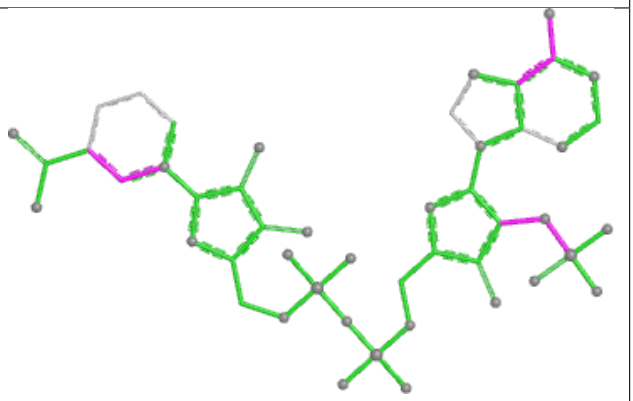


Rings

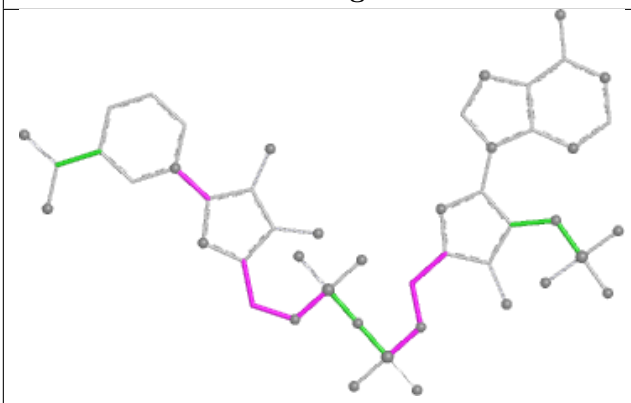
Ligand NDP B 2602



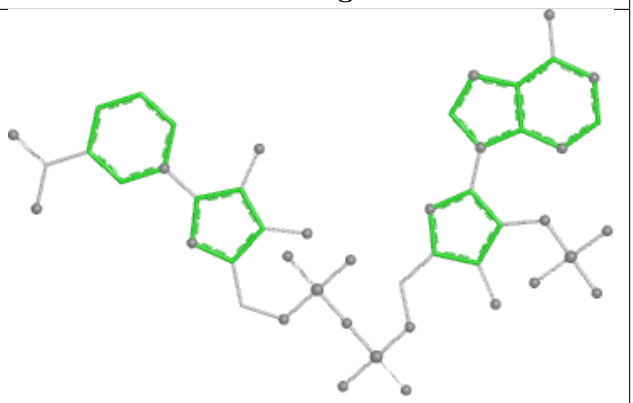
Bond lengths



Bond angles

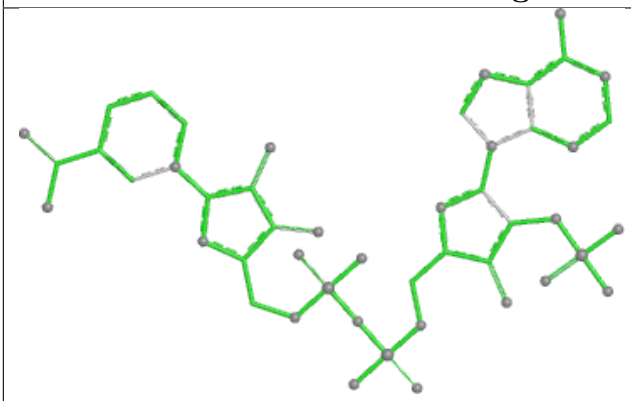


Torsions

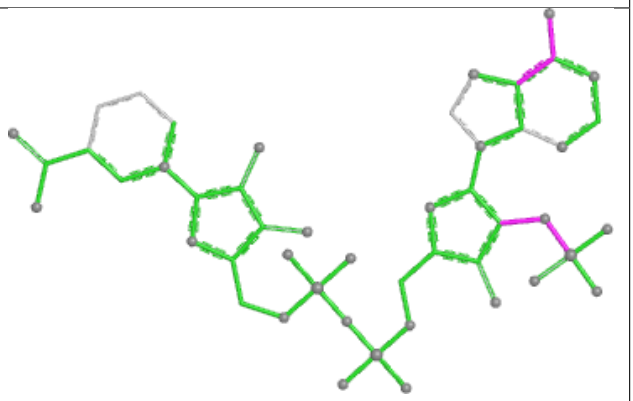


Rings

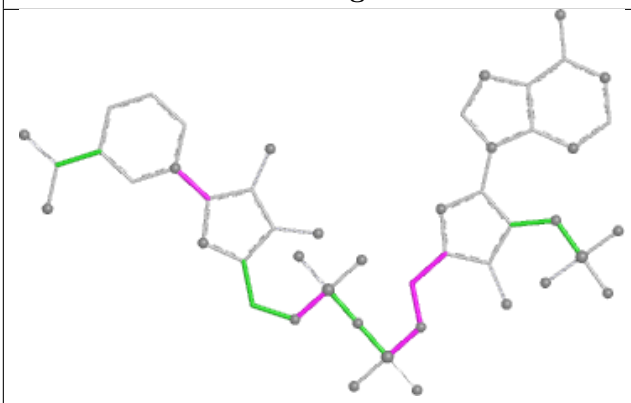
Ligand NDP A 2602



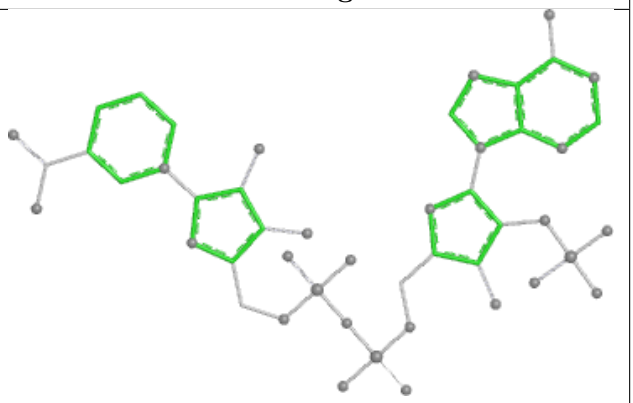
Bond lengths



Bond angles

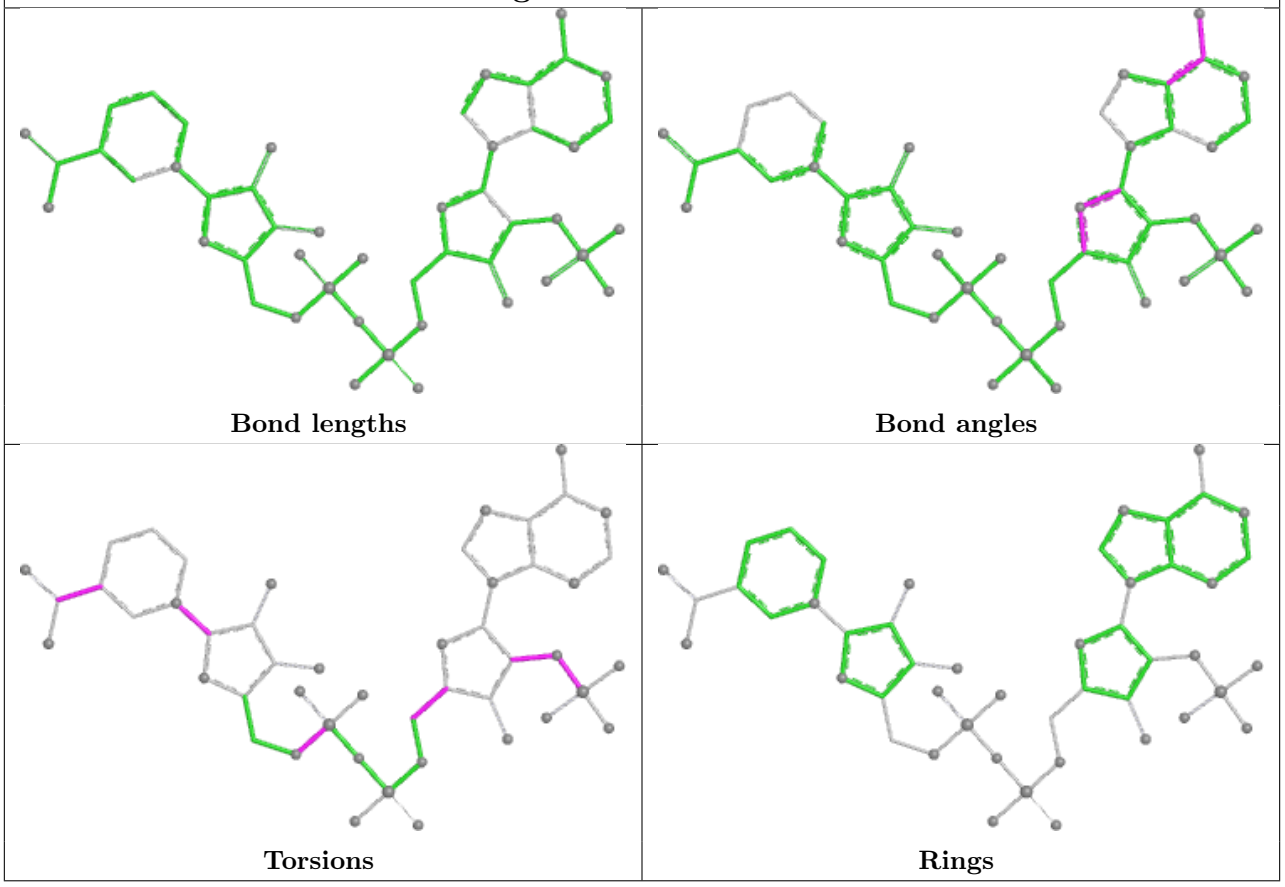


Torsions



Rings

Ligand NDP A 2601



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.

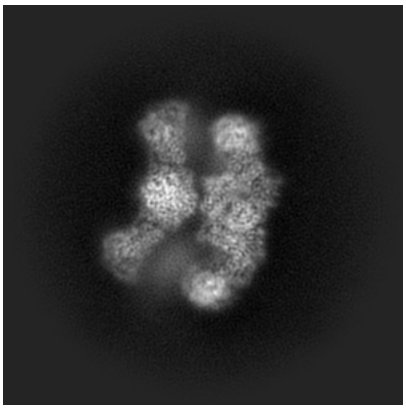
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43341. These allow visual inspection of the internal detail of the map and identification of artifacts.

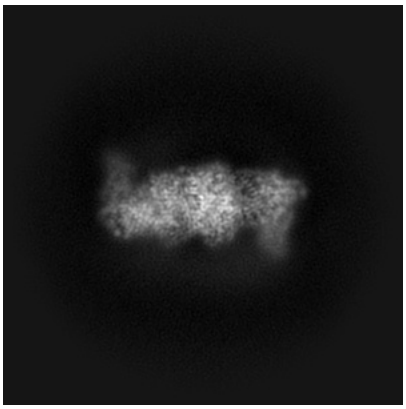
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

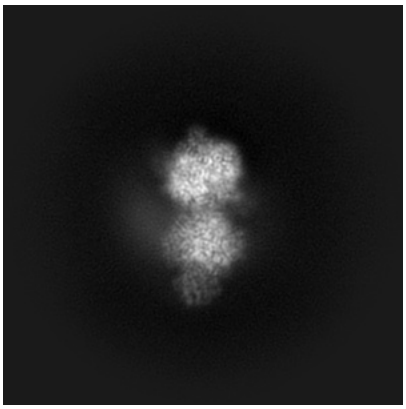
6.1.1 Primary map



X

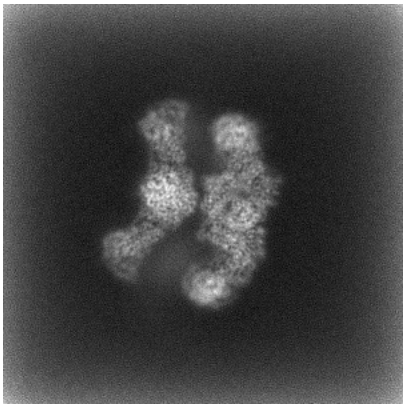


Y

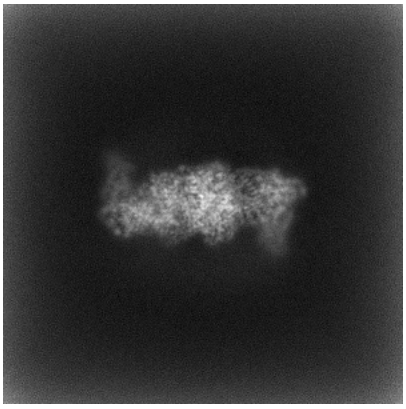


Z

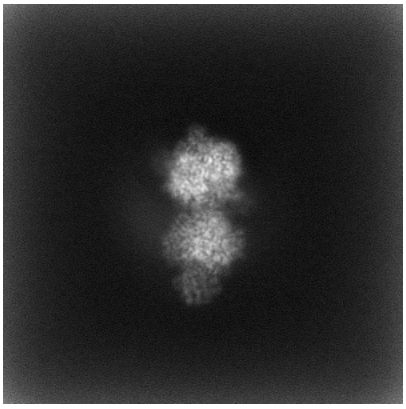
6.1.2 Raw map



X



Y

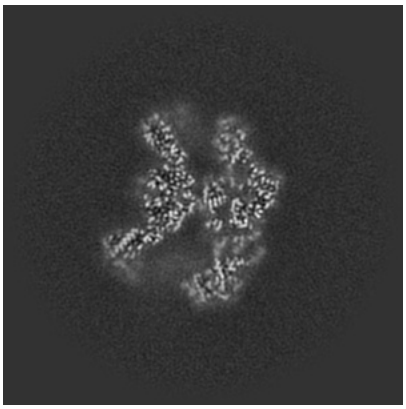


Z

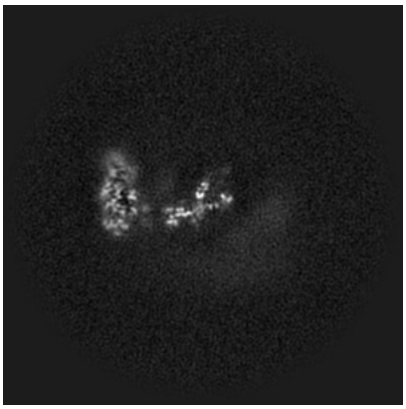
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

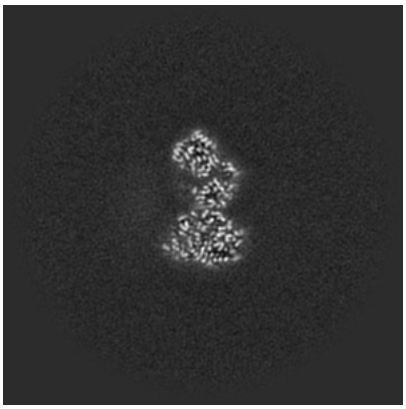
6.2.1 Primary map



X Index: 180

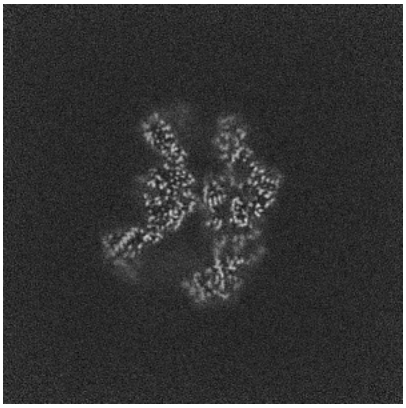


Y Index: 180

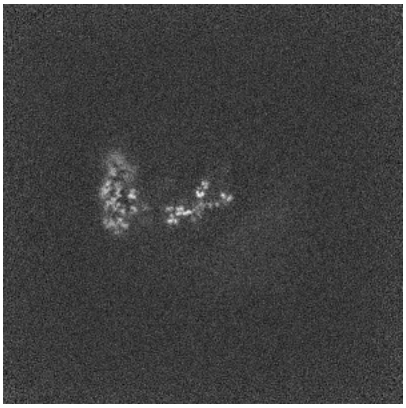


Z Index: 180

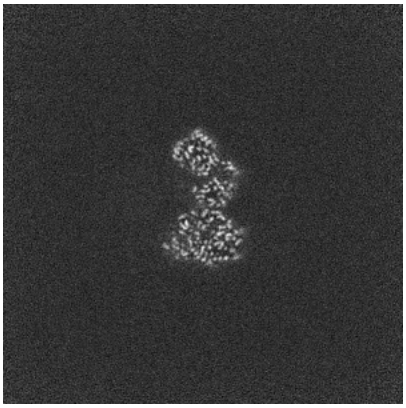
6.2.2 Raw map



X Index: 180



Y Index: 180

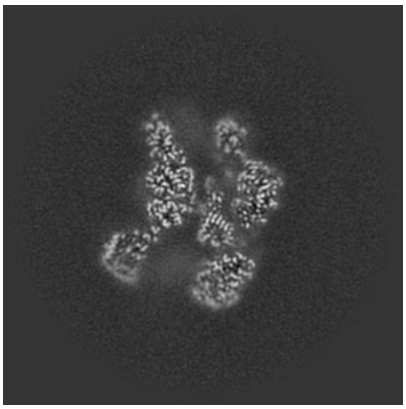


Z Index: 180

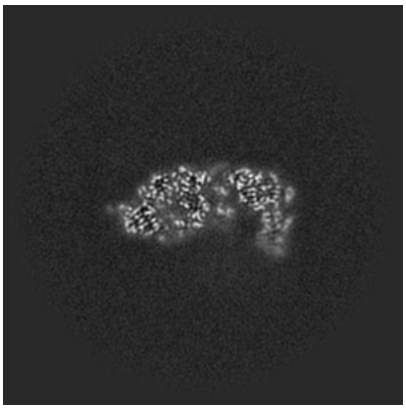
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

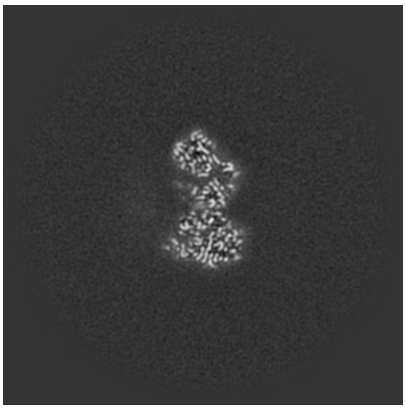
6.3.1 Primary map



X Index: 175

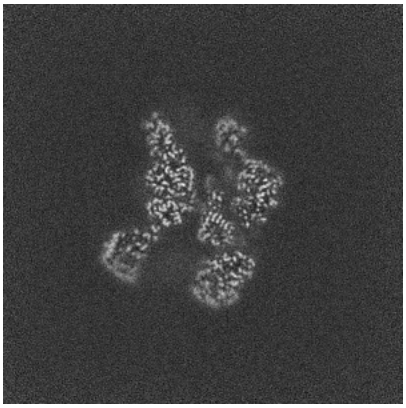


Y Index: 212

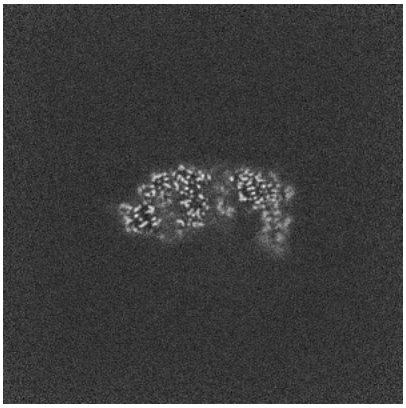


Z Index: 179

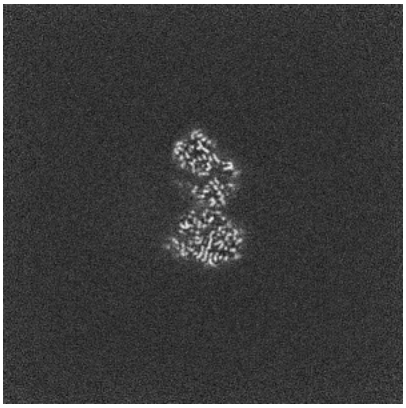
6.3.2 Raw map



X Index: 175



Y Index: 213

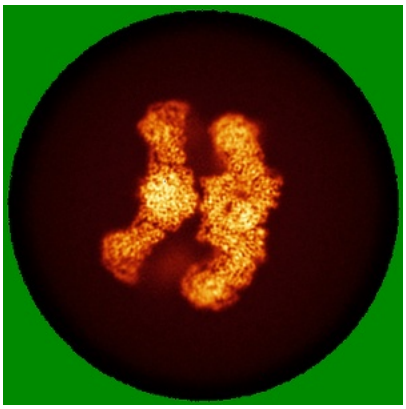


Z Index: 179

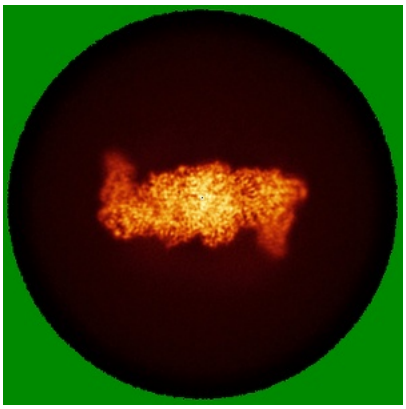
The images above show the largest variance slices of the map in three orthogonal directions.

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

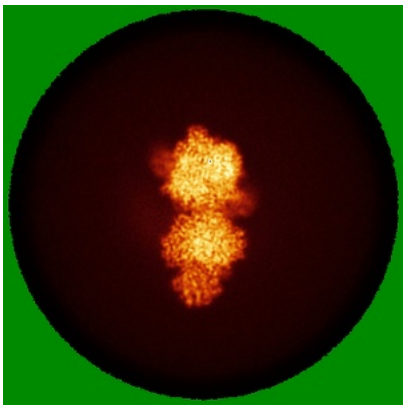
6.4.1 Primary map



X

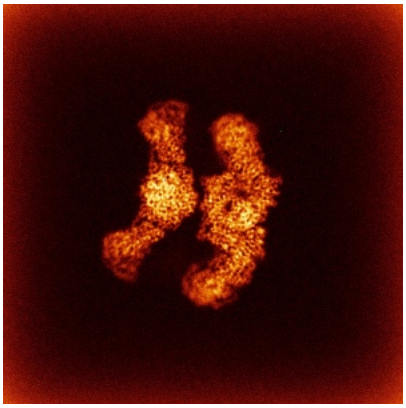


Y

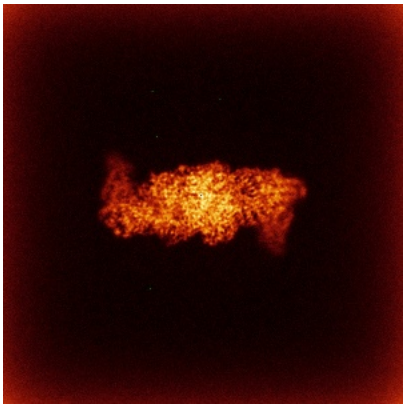


Z

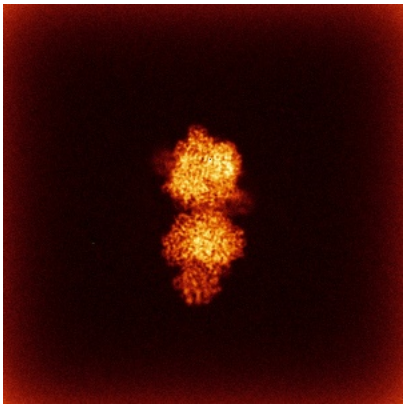
6.4.2 Raw map



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)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.197. 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.

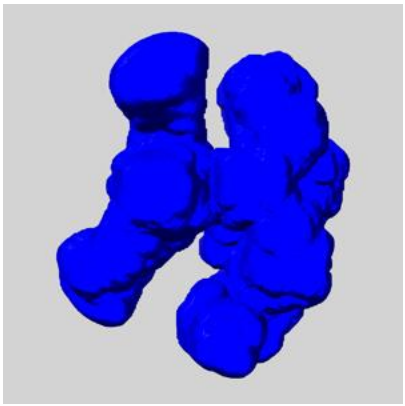
6.6 Mask visualisation

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

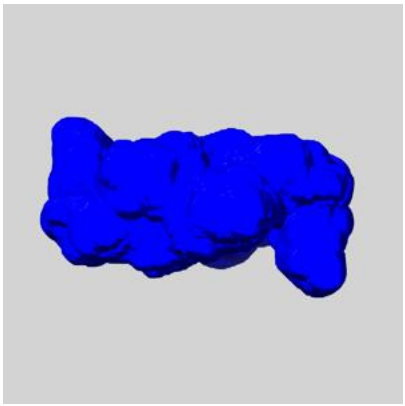
A mask typically either:

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

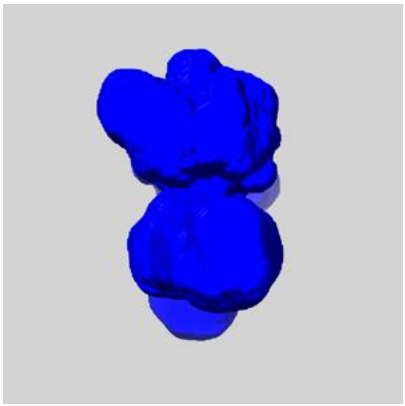
6.6.1 emd_43341_msk_1.map



X



Y

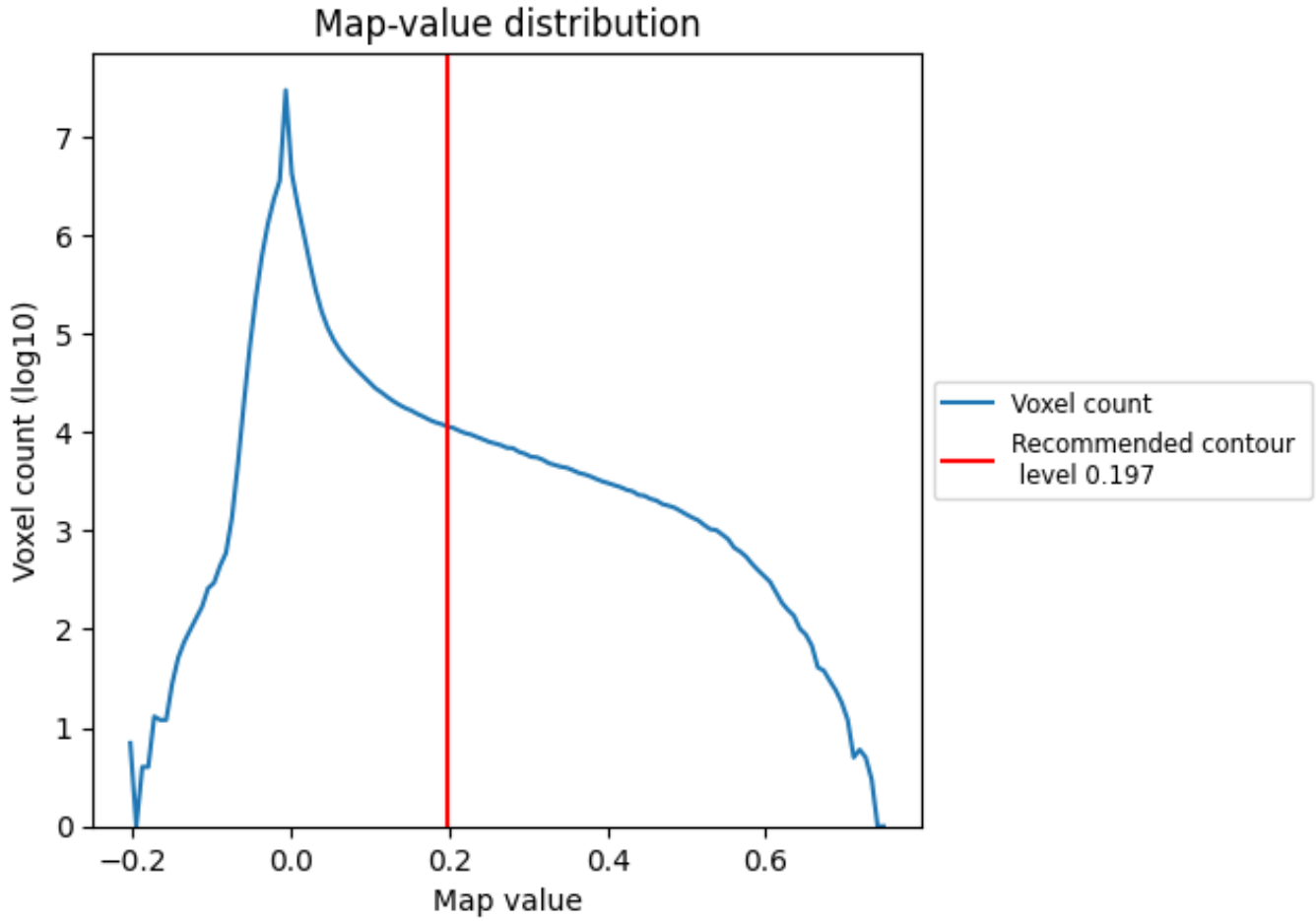


Z

7 Map analysis

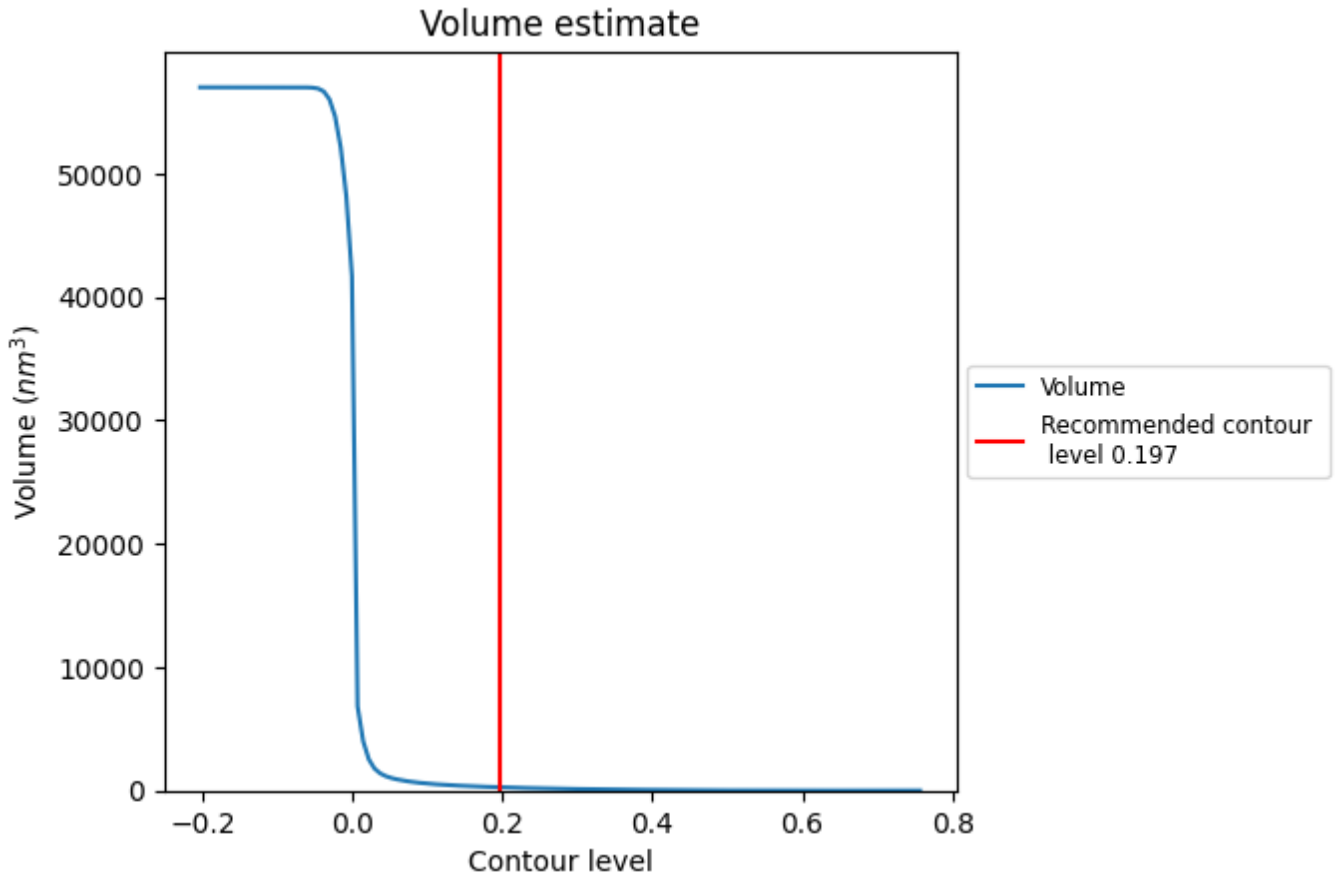
This section contains the results of statistical analysis of the map.

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.

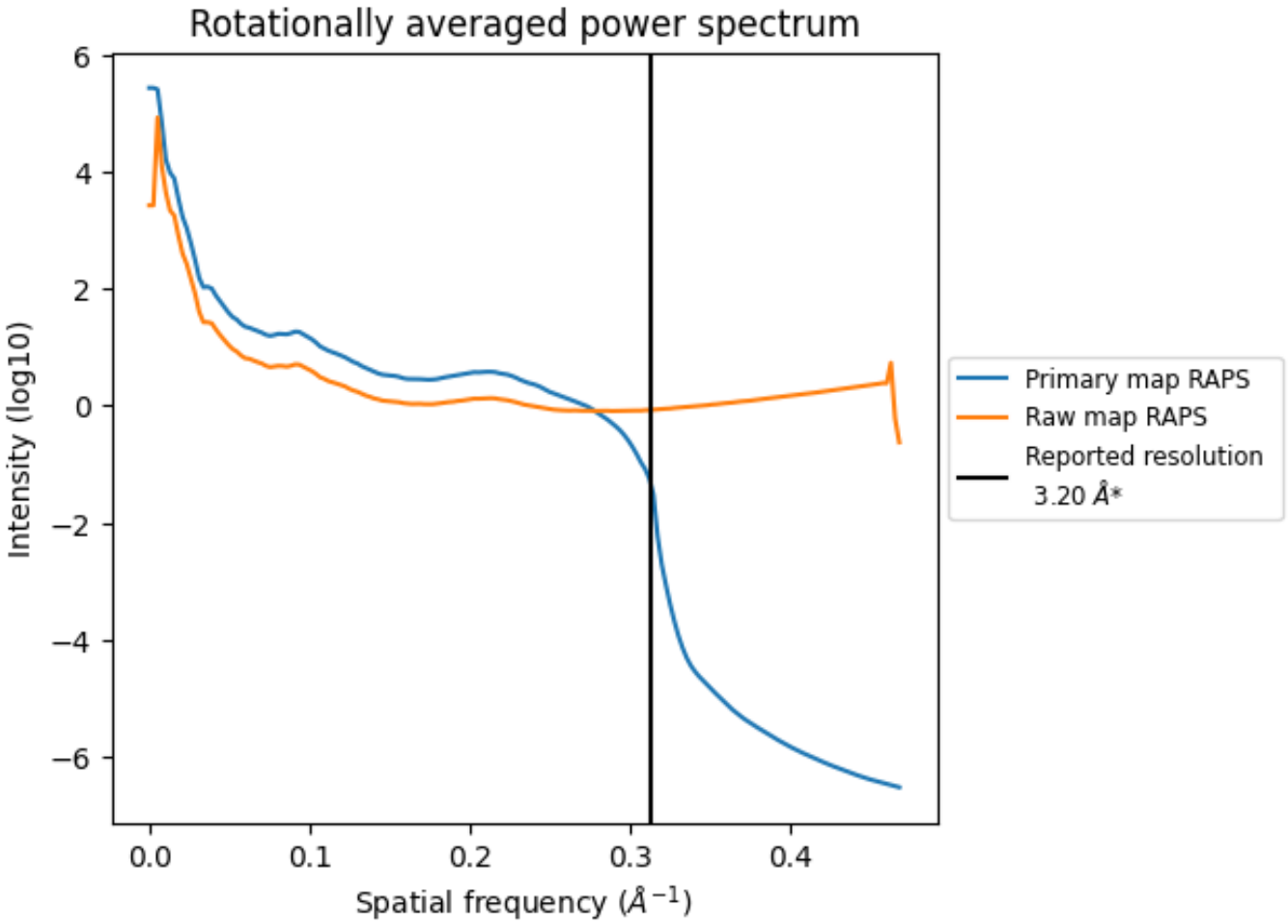
7.2 Volume estimate



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 241 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

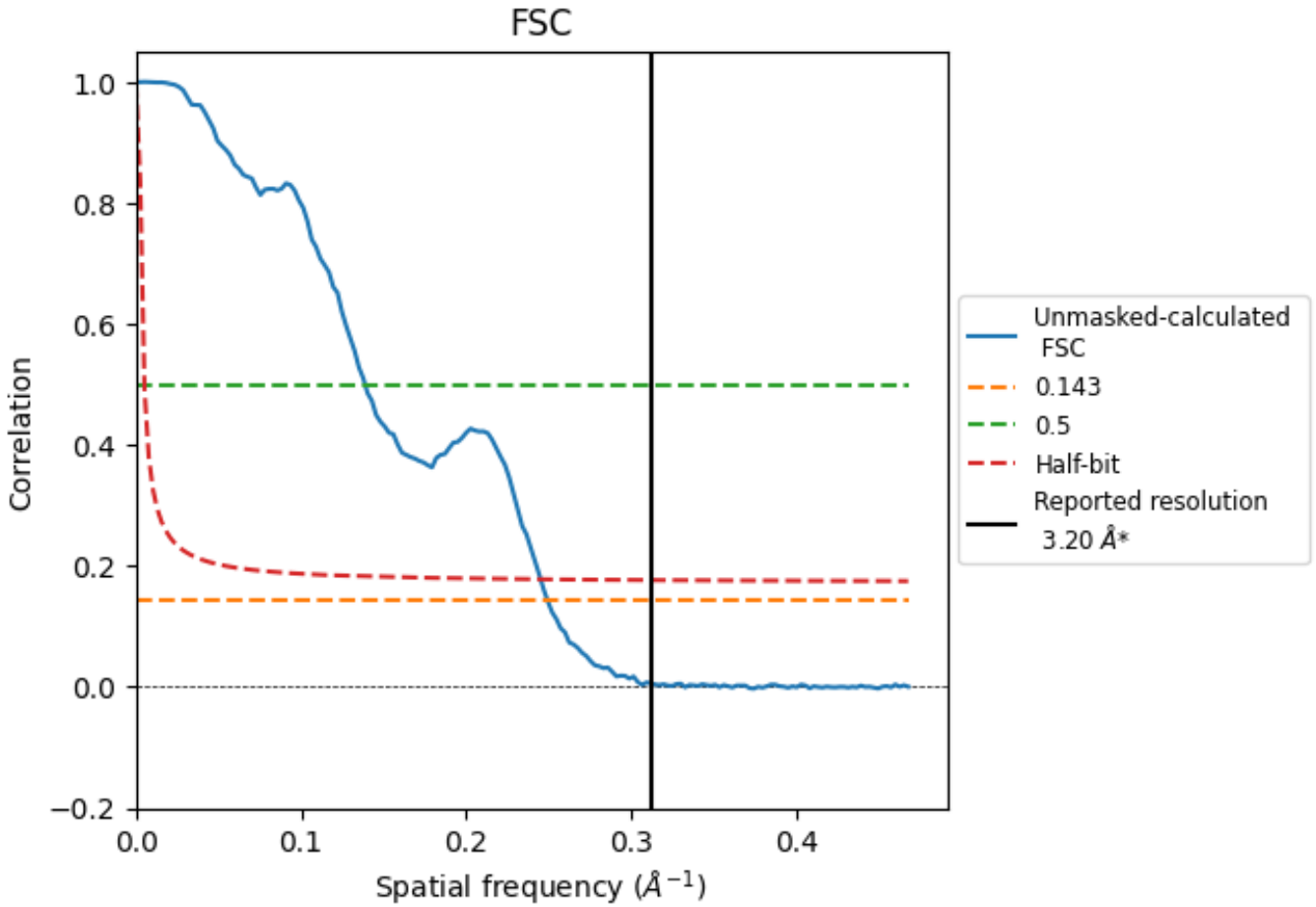


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

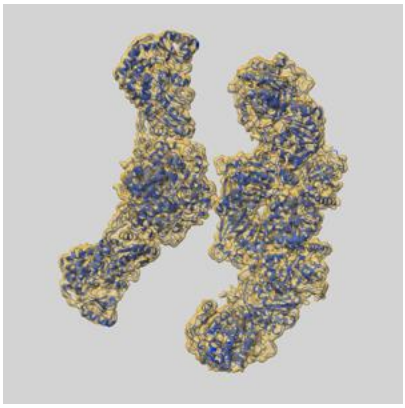
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.20	4.08

*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 4.01 differs from the reported value 3.2 by more than 10 %

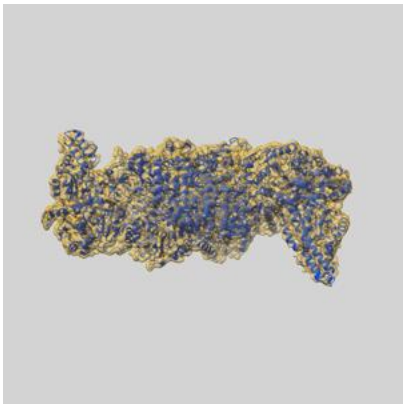
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43341 and PDB model 8VLP. Per-residue inclusion information can be found in section 3 on page 7.

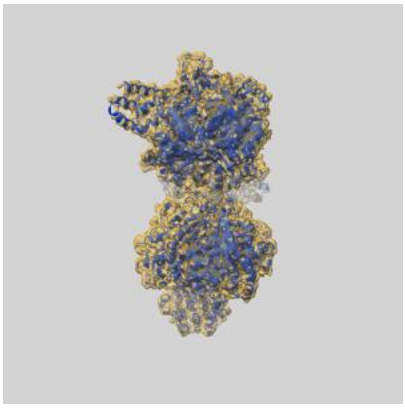
9.1 Map-model overlay



X



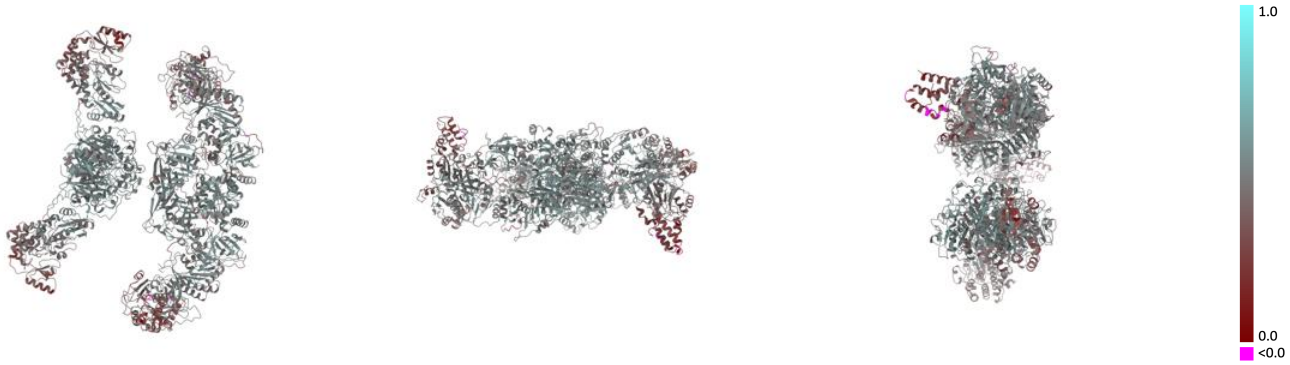
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.197 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

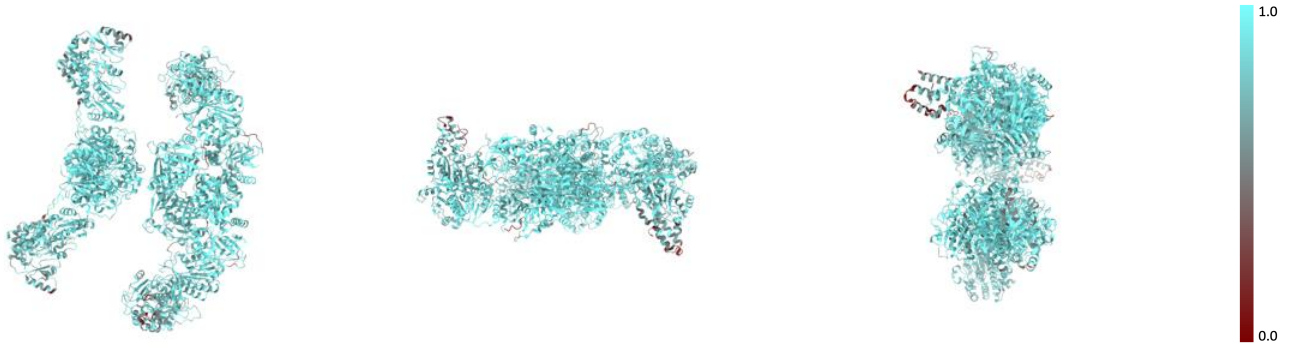
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

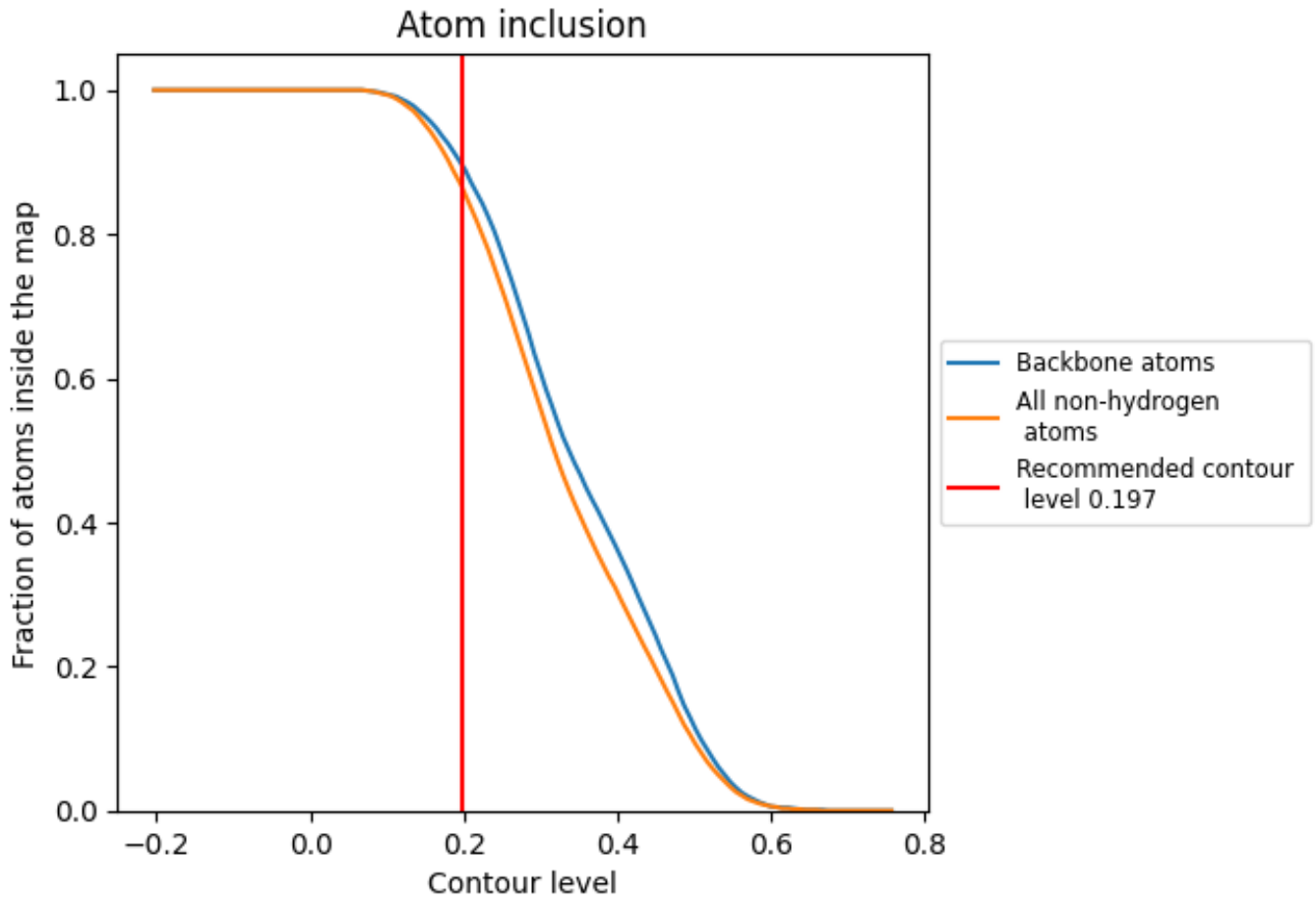
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.197).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.4740
A	0.8690	0.4750
B	0.8650	0.4730