WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 03:55 PM EST

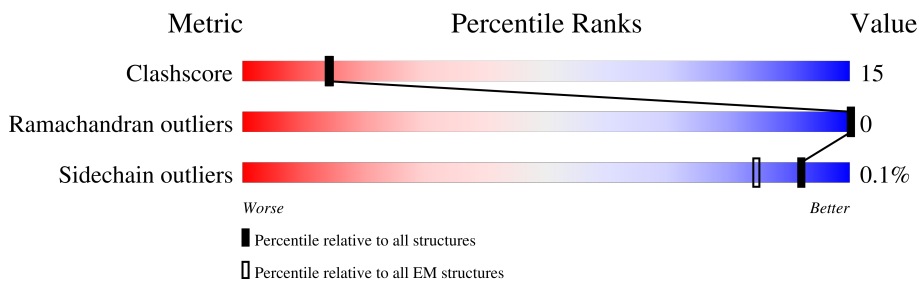|		
PDB ID	:	8VLE
EMDB ID	:	EMD-43337
Title	:	Composite structure of human FASN with NADPH in State 1
Authors	:	Schultz, K.; Marmorstein, R.
Deposited on	:	2024-01-11
Resolution	:	3.30 Å(reported)
Based on initial models	:	., 3HHD

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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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		0
Sidechain outliers		0.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 ⓘ

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 25182	C 10041	H 9349	N 2785	O 2934	S 73	0	0
1	B	2071	Total 25237	C 10054	H 9380	N 2789	O 2941	S 73	0	0

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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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
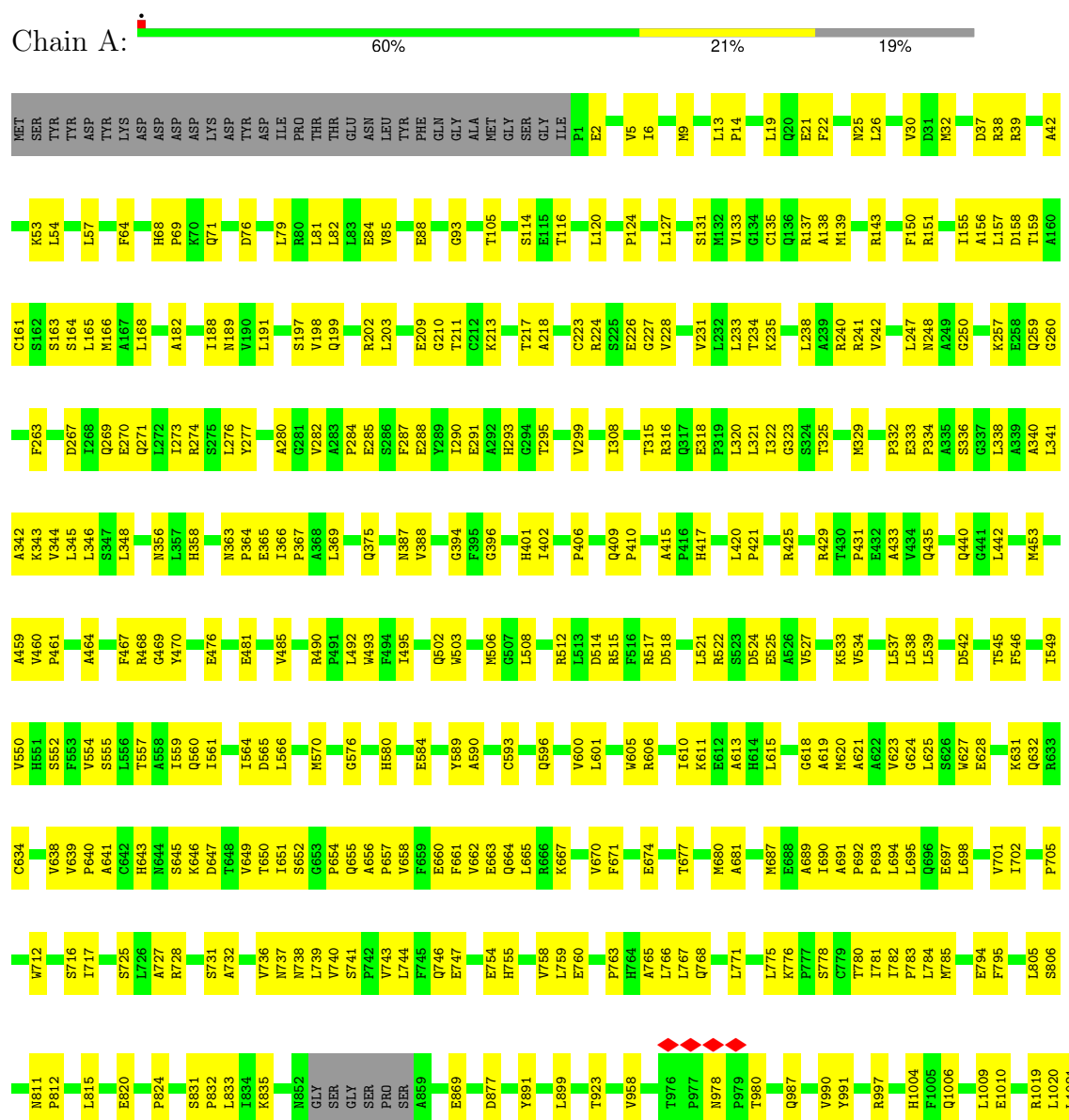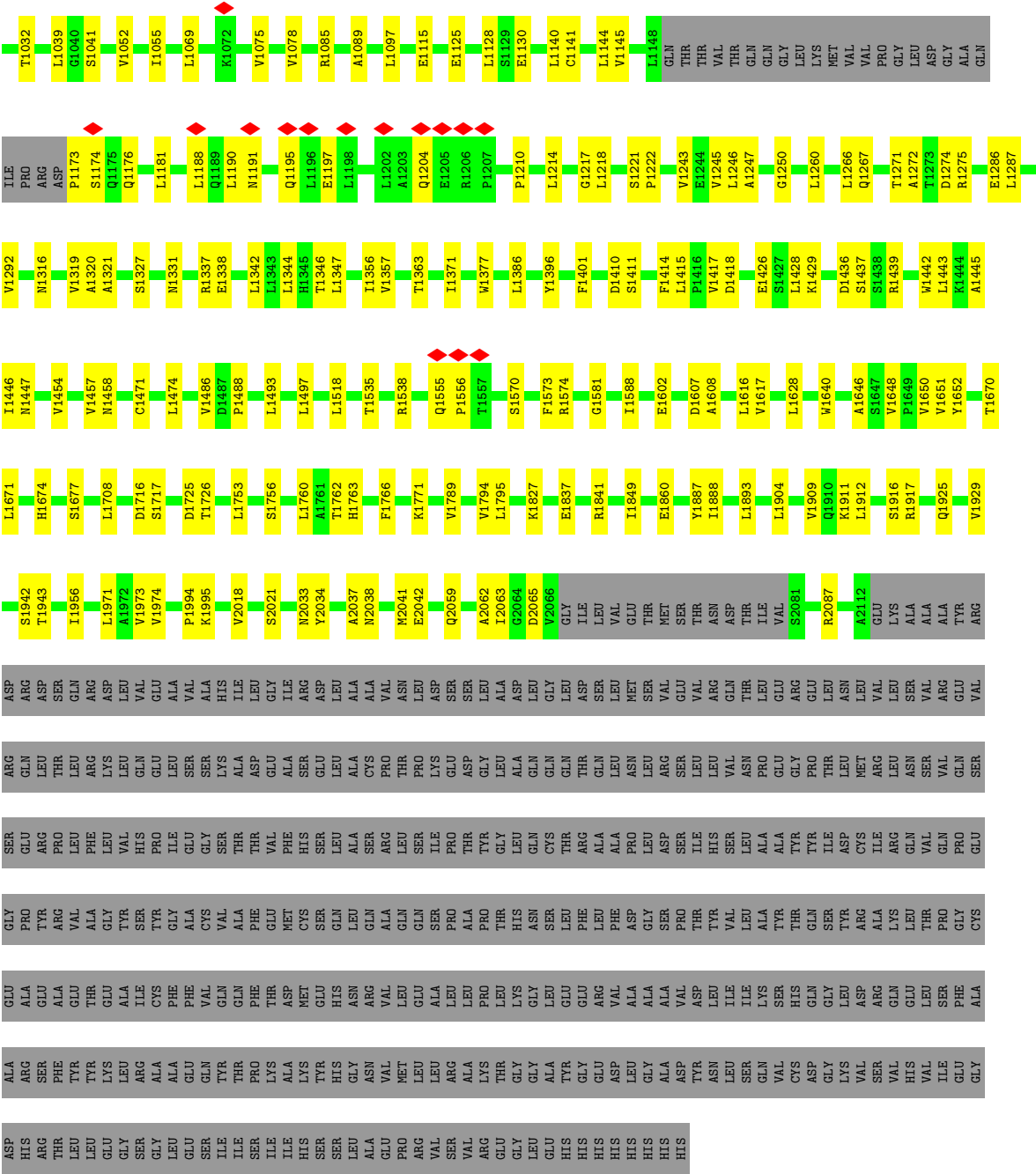

NDP
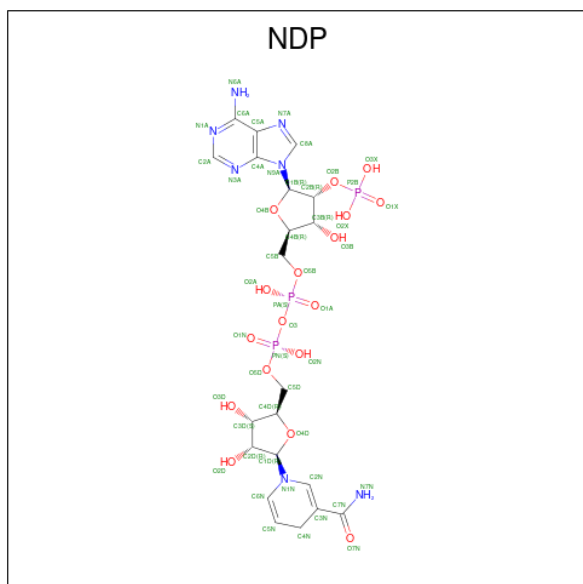
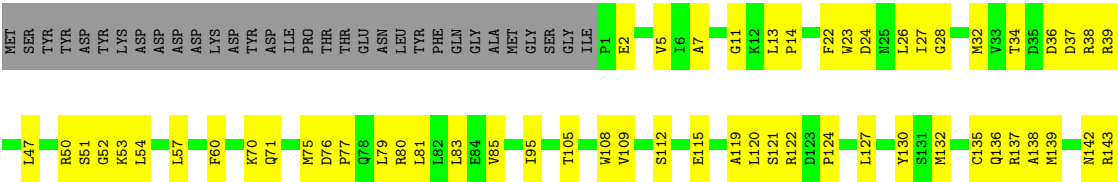| Mol	Chain	Residues	Atoms							AltConf
2	A	1	Total	C	H	N	O	P		0
			74	21	26	7	17	3		
2	A	1	Total	C	H	N	O	P		0
			74	21	26	7	17	3		
2	B	1	Total	C	H	N	O	P		0
			74	21	26	7	17	3		
2	B	1	Total	C	H	N	O	P		0
			74	21	26	7	17	3		

3　Residue-property plots ⓘ

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

This is a full-page figure showing residue-level validation data for Molecule 1: Fatty acid synthase. The figure consists of rows of colored residue boxes (green, yellow, grey) with red diamond markers above some residues.

Row 1: T1032 L1039 G1040 S1041 V1052 I1065 L1069 K1072 V1075 V1078 R1085 A1089 L1097 E1115 E1125 E1130 L1128 S1129 L1140 C1141 L1144 V1145 L1148 GLN THR THR VAL THR GLN GLN GLY LEU LYS MET VAL VAL PRO GLY LEU ASP GLY ALA GLN

Row 2: ILE PRO ARG ASP P1173 S1174 Q1175 Q1176 L1181 L1188 Q1189 L1190 N1191 Q1195 L1196 E1197 L1198 L1202 A1203 Q1204 E1205 R1206 P1207 P1210 L1214 G1217 L1218 S1221 P1222 V1243 E1244 V1245 L1246 A1247 G1250 L1260 L1266 Q1267 T1271 A1272 T1273 D1274 R1275 E1286 L1287

Row 3: V1292 N1316 V1319 A1320 A1321 S1327 N1331 R1337 E1338 L1342 L1343 L1344 H1345 T1346 L1347 I1356 V1357 T1363 I1371 W1377 L1386 Y1396 F1401 D1410 S1411 F1414 L1415 P1416 V1417 D1418 E1426 S1427 L1428 K1429 D1436 S1437 S1438 R1439 W1442 L1443 K1444 A1445

Row 4: I1446 N1447 V1454 V1457 N1458 C1471 L1474 V1486 D1487 P1488 L1493 L1497 L1518 T1535 R1538 Q1555 P1556 T1557 S1570 F1573 R1574 G1581 I1588 E1602 D1607 A1608 L1616 V1617 L1628 W1640 A1646 S1647 V1648 P1649 V1650 V1651 Y1652 T1670

Row 5: L1671 H1674 S1677 L1708 D1716 S1717 D1725 T1726 L1753 S1756 L1760 A1761 T1762 H1763 F1766 K1771 V1789 V1794 L1795 K1827 E1837 R1841 I1849 E1860 Y1887 I1888 L1893 L1904 V1909 Q1910 K1911 L1912 S1916 R1917 Q1925 V1929

Row 6: S1942 T1943 I1956 L1971 A1972 V1973 V1974 P1994 K1995 V2018 S2021 N2033 Y2034 A2037 N2038 M2041 E2042 Q2059 A2062 I2063 G2064 D2065 V2066 GLY ILE LEU VAL GLU THR MET SER THR ASN ASP THR ILE VAL S2081 R2087 A2112 GLU LYS ALA ALA ALA TYR ARG

Row 7: ASP ARG ASP SER GLN ARG ASP LEU VAL GLU ALA VAL ALA HIS ILE LEU GLY ILE ARG ASP SER GLU SER SER LEU ALA ASP GLY LEU ASP SER SER LEU MET SER VAL GLU VAL ARG GLN THR LEU GLU ARG GLU LEU ASN LEU VAL LEU SER VAL ARG GLU VAL

Row 8: ARG GLN LEU THR LEU ARG LYS LEU GLN LEU SER LYS ALA ASP GLU ALA SER GLU LEU ALA CYS PRO THR PRO LYS GLU GLU ASP GLY LEU ALA GLN GLN GLN SER PRO ALA PRO THR HIS ASN SER LEU PHE LEU ASP GLY SER PRO THR TYR VAL LEU ALA TYR THR GLN SER TYR ILE ASP CYS ILE ARG GLN GLN VAL GLN PRO GLU

Row 9: SER GLU ARG PRO LEU PHE VAL LEU HIS PRO ILE GLU GLY PHE VAL CYS VAL ALA ASP PHE HIS ILE LEU SER ARG LEU ALA SER ILE PRO THR TYR GLY LEU GLN ASP CYS THR ARG ALA ALA ALA VAL ASP TYR LEU ILE ILE LYS SER HIS GLN LEU GLU ASP SER CYS ILE ARG GLN GLN VAL LEU THR PRO GLY CYS

Row 10: GLY PRO TYR ARG VAL ALA GLY TYR SER TYR GLY ALA CYS VAL ALA PHE GLU MET CYS SER GLN LEU GLN ALA GLN GLN SER PRO ALA PRO THR HIS ASN SER LEU PHE LEU ASP GLY SER GLY ALA TYR GLY LEU GLU GLU ARG VAL ALA ALA ALA VAL ASP TYR LEU ILE ILE LYS SER HIS GLY LEU GLU GLN LEU THR PRO GLY CYS

Row 11: GLU ALA GLU ALA GLU THR GLU ALA ILE CYS PHE PHE VAL GLN GLN PHE THR THR ASP MET GLU HIS ASN ARG VAL LEU GLU ALA ALA GLN SER TYR TYR THR GLN LEU SER ASP TYR ARG ALA LYS LEU GLU THR PRO GLY CYS PHE ILE LEU ILE LYS SER HIS GLN LEU GLU ASP SER PHE ALA

Row 12: ALA ARG SER PHE TYR TYR LYS LEU ARG ALA ALA GLU GLN SER VAL CYS TYR THR PRO LYS ALA LYS VAL HIS GLY ASN VAL MET LEU LEU ARG ALA LYS THR GLY GLY ALA TYR GLY GLU GLU LEU GLY ARG VAL ALA ALA ALA VAL ASP TYR LEU ILE ILE LYS SER HIS VAL CYS ASP GLY LYS VAL SER VAL HIS ILE GLU GLY

Row 13: ASP HIS ARG THR LEU LEU GLU GLY GLY SER LEU LEU GLU SER ILE ILE HIS SER ILE LEU ALA GLU PRO ARG VAL SER VAL ARG GLU GLY LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Fatty acid synthase

Chain B:
60%　　21%　　19%

Chain B Row 1: MET SER TYR TYR ASP TYR LYS ASP ASP ASP LYS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET GLY SER GLY ILE P1 E2 V5 I6 A7 G11 K12 L13 P14 F22 W23 D24 N25 L26 I27 G28 M32 V33 T34 D35 D36 D37 R38 R39

Chain B Row 2: 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

VAL LEU SER VAL ARG GLU VAL ARG GLN LEU THR LEU ARG ARG LYS LEU GLN GLU LEU GLU LEU SER SER LYS ALA ASP GLU ALA SER GLU LEU ALA CYS PRO THR PRO LYS GLU ASP GLY LEU ALA GLN GLN THR GLN LEU ASN ARG 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 SER LEU ALA SER ARG LEU SER ILE PRO THR GLY TYR GLY LEU GLN CYS THR ARG ALA ALA PRO LEU ASP SER ILE HIS SER LEU ALA ALA TYR TYR ILE ASP CYS

ILE ARG GLN VAL GLN PRO GLY PRO GLY PRO TYR ARG VAL ALA GLY TYR SER TYR GLY ALA CYS VAL ALA PHE GLU MET CYS SER GLN LEU GLN ALA GLN GLN SER PRO ALA 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 GLY THR ALA ILE CYS PHE PHE VAL GLN GLN PHE THR ASP MET GLU HIS ASN ARG VAL LEU GLU GLU ALA LEU LEU PRO LEU LYS GLY LEU GLU GLU ARG VAL 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 THR TYR PRO LYS ALA LYS LYS TYR HIS GLY ASN VAL MET LEU LEU ARG ALA LYS THR GLY GLY ALA TYR GLU GLU ASP GLY SER LEU ALA ALA ASP TYR ASN LEU SER GLN VAL CYS ASP GLY LYS LEU VAL

SER VAL HIS VAL ILE GLU GLY ASP HIS ARG THR LEU LEU GLU GLY SER GLY LEU GLU GLU SER ILE ILE HIS SER ILE LEU HIS SER SER LEU ALA GLU PRO ARG ALA VAL SER VAL ARG GLU GLY GLY LEU GLU 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 $(e^-/\text{Å}^2)$	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 (i)

5.1   Standard geometry (i)

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	0.26	0/16198	0.48	0/22023
1	B	0.27	0/16222	0.48	0/22055
All	All	0.26	0/32420	0.48	0/44078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9349	15809	507	0
1	B	15857	9380	15826	478	0
2	A	96	52	52	23	0
2	B	96	52	52	11	0
All	All	31882	18833	31739	974	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (974) 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: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:570:MET:HE2	1:A:815:LEU:HD11	1.51	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: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: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:2021:SER:OG	2:A:2602:NDP:H5N	1.79	0.81
1:A:570:MET:HE3	1:A:815:LEU:HD21	1.62	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:139:MET:HE2	1:A:139:MET:HA	1.68	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:624:GLY:HA3	1:A:671:PHE:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1141:CYS:O	1:A:1145:VAL:HG23	1.99	0.62
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: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:B:1652:TYR:OH	1:B:1824:ARG:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HB3	1:B:372:GLY:O	2.01	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:B:620:MET:HE1	1:B:682:PHE:HB2	1.83	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
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: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:A:1942:SER:O	1:A:1943:THR:OG1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:329:MET:HE1	1:A:332:PRO:HG3	1.84	0.59
1:B:325:THR:HB	1:B:343:LYS:CD	2.32	0.59
1:B:620:MET:CE	1:B:682:PHE:HB2	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: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
1:A:139:MET:HE2	1:A:139:MET:CA	2.33	0.58
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: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:687:MET:HE2	1:A:739:LEU:HD11	1.85	0.57
1:A:987:GLN:NE2	1:A:1006:GLN:O	2.37	0.57
1:B:576:GLY:C	1:B:577:ILE:HD12	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:1535:THR:HG23	1:A:1535:THR:O	2.06	0.55
1:B:333:GLU:CB	1:B:334:PRO:HD3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:687:MET:CE	1:A:739:LEU:HD11	2.37	0.55
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: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:610:ILE:HG12	1:B:687:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1128:LEU:HD21	1:A:1217:GLY:C	2.30	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:1973:VAL:H	2:A:2602:NDP:H52A	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:624:GLY:CA	1:A:671:PHE:HB3	2.39	0.52
1:B:511:MET:HE2	1:B:520:ILE:HG21	1.91	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:533:LYS:O	1:A:537:LEU:HG	2.10	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:191:LEU:C	1:B:192:LEU:HD12	2.31	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: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: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:1972:ALA:HB1	2:B:2602:NDP:C5A	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:615:LEU:HB2	1:A:680:MET:CE	2.41	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
1:A:39:ARG:HG2	1:A:53:LYS:HD2	1.93	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:A:780:THR:C	1:A:781:ILE:HD12	2.31	0.51
1:B:325:THR:HG21	1:B:340:ALA:HA	1.93	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:A:1245:VAL:C	1:A:1246:LEU:HD12	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:628:GLU:H	1:B:628:GLU:CD	2.13	0.50
1:A:188:ILE:HG22	1:A:228:VAL:HG13	1.93	0.49
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: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:615:LEU:HD21	1:B:680:MET:HE3	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:B:213:LYS:HG2	1:B:358:HIS:HB3	1.93	0.49
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:879:THR:C	1:B:880:LEU:HD12	2.33	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: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: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:621:ALA:O	1:B:651:ILE:N	2.40	0.48
1:B:1371:ILE:C	1:B:1372:LEU:HD12	2.33	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:502:GLN:HB2	1:A:506:MET:HE2	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:763:PRO:HA	1:A:785:MET:HE1	1.96	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1794:VAL:C	1:A:1795:LEU:HD23	2.35	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:B:1214:LEU:HD12	1:B:1214:LEU:C	2.35	0.47
1:A:442:LEU:HD23	1:A:442:LEU:C	2.35	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: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:1021:LEU:HD23	1:A:1075:VAL:HG12	1.95	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:105:THR:HG23	1:A:182:ALA:C	2.36	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: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:615:LEU:HB2	1:A:680:MET:HE3	1.97	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: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: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: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:34:THR:O	1:B:50:ARG:HA	2.16	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:499:MET:HE2	1:B:582:LEU:HB2	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: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
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:A:978:ASN:C	1:A:980:THR:HG23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:1753:LEU:C	1:A:1753:LEU:HD23	2.38	0.44
1:B:489:GLU:HA	1:B:489:GLU:OE1	2.18	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:127:LEU:HD12	1:A:127:LEU:C	2.38	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
1:B:2:GLU:OE1	1:B:2:GLU:HA	2.17	0.44
1:B:112:SER:C	1:B:137:ARG:HH21	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:PRO:O	1:A:32:MET:HE1	2.17	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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:155:ILE:HG22	1:A:156:ALA:N	2.34	0.42
1:A:203:LEU:HD12	1:B:132:MET:HE2	2.00	0.42
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
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: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: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:B:499:MET:HE3	1:B:582:LEU:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:1346:THR:HG22	1:A:1347:LEU:N	2.35	0.42
1:B:766:LEU:HD23	1:B:766:LEU:C	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:760:GLU:CD	1:A:765:ALA:HA	2.40	0.41
1:A:1670:THR:C	1:A:1671:LEU:HD12	2.41	0.41
1:A:1771:LYS:HE2	1:A:1795:LEU:HD22	2.02	0.41
1:B:168:LEU:HD23	1:B:168:LEU:C	2.40	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
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:351:GLY:C	1:B:352:LEU:HD12	2.41	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:241:ARG:HD2	1:A:453:MET:HE1	2.03	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:139:MET:HA	1:A:139:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2097:LEU:HD23	1:B:2097:LEU:C	2.41	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: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: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: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: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:763:PRO:HA	1:A:785:MET:CE	2.50	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
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:A:1674:HIS:NE2	1:A:1756:SER:OG	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1445:ALA:C	1:B:1446:ILE:HD13	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:639:VAL:CG1	1:B:640:PRO:HD2	2.46	0.40
1:A:549:ILE:O	1:A:552:SER:OG	2.32	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:654:PRO:O	1:A:658:VAL:HG23	2.21	0.40
1:B:497:SER:HB3	1:B:762:ALA:HB2	2.02	0.40
1:B:1461:ARG:HD2	1:B:1502:VAL:HG21	2.03	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:1426:GLU:OE1	1:A:1429:LYS:NZ	2.44	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	1703 (100%)	5 (0%)	91	94
All	All	3413/4234 (81%)	3408 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	378	ASP
1	B	782	ILE
1	B	1211	GLU
1	B	1801	ASN
1	B	1802	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	170	ASN
1	A	173	GLN
1	A	328	ASN
1	A	356	ASN

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Mol	Chain	Res	Type
1	A	379	GLN
1	A	387	ASN
1	A	399	ASN
1	A	446	GLN
1	A	738	ASN
1	A	746	GLN
1	A	863	ASN
1	A	987	GLN
1	A	1139	GLN
1	A	1191	ASN
1	A	1296	GLN
1	A	1504	ASN
1	A	1595	GLN
1	A	1835	GLN
1	A	2001	ASN
1	A	2028	ASN
1	A	2101	GLN
1	B	142	ASN
1	B	173	GLN
1	B	199	GLN
1	B	293	HIS
1	B	356	ASN
1	B	375	GLN
1	B	399	ASN
1	B	440	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	1056	HIS
1	B	1294	GLN
1	B	1331	ASN
1	B	1345	HIS
1	B	1369	GLN
1	B	1722	ASN
1	B	1815	GLN
1	B	1835	GLN

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Mol	Chain	Res	Type
1	B	1845	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	A	2602	-	47,52,52	0.64	0	61,80,80	0.90	3 (4%)
2	NDP	B	2601	-	47,52,52	0.67	0	61,80,80	0.82	2 (3%)
2	NDP	A	2601	-	47,52,52	0.68	0	61,80,80	0.81	2 (3%)
2	NDP	B	2602	-	47,52,52	0.64	0	61,80,80	0.90	3 (4%)

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

There are no bond length outliers.

All (10) 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	B	2601	NDP	C5A-C6A-N6A	2.30	123.82	120.31
2	A	2602	NDP	C5A-C6A-N6A	2.30	123.81	120.31
2	B	2602	NDP	C5A-C6A-N6A	2.16	123.61	120.31
2	A	2602	NDP	C3N-C2N-N1N	-2.14	120.06	123.20
2	A	2601	NDP	C5A-C6A-N6A	2.10	123.51	120.31
2	A	2601	NDP	O4D-C1D-C2D	-2.08	102.17	106.62

There are no chirality outliers.

All (39) 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

Continued on next page...

Continued from previous page...

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	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	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	A	2602	NDP	20	0
2	B	2601	NDP	2	0
2	A	2601	NDP	3	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 A 2602

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 2601

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 2601

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 2602

Bond lengths

Bond angles

Torsions

Rings
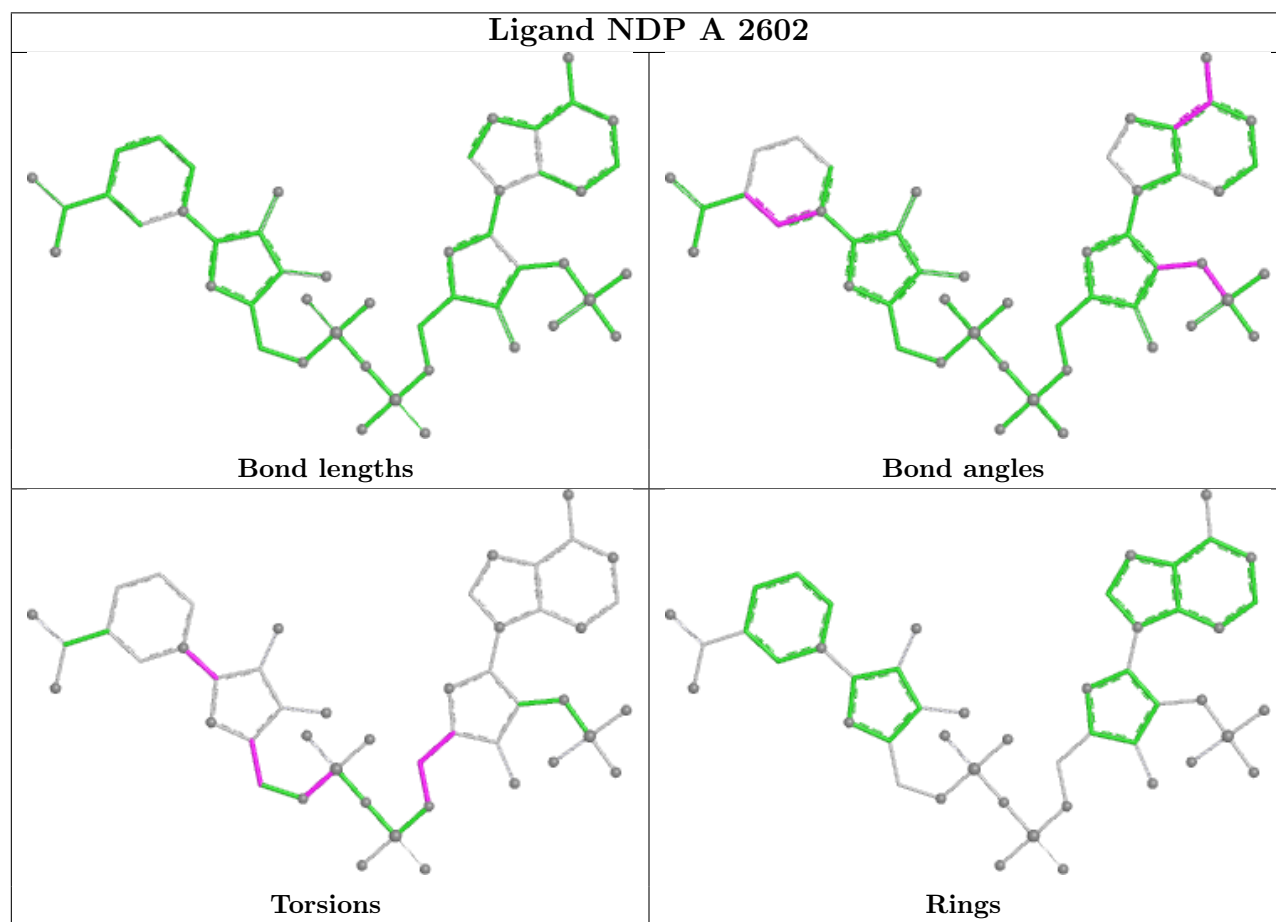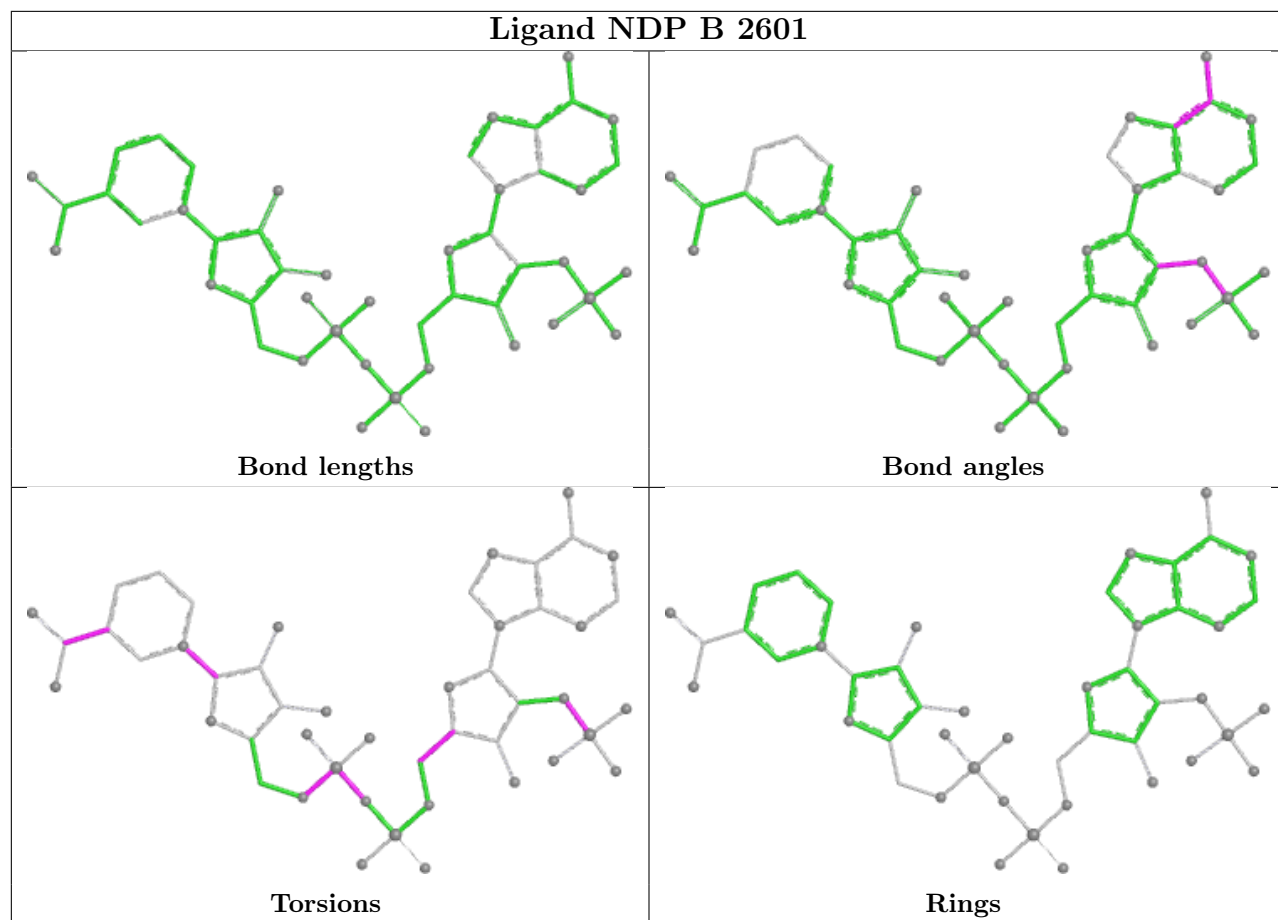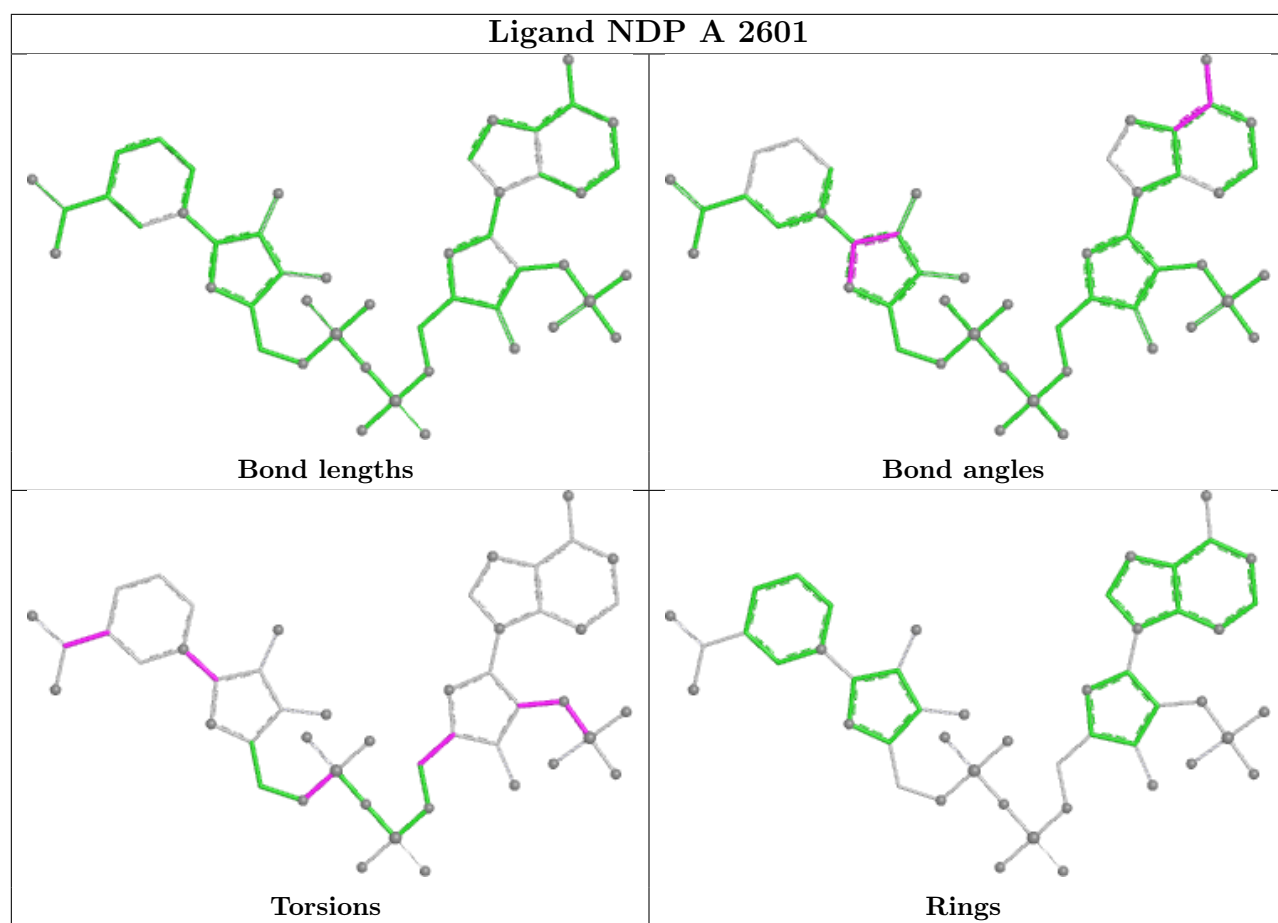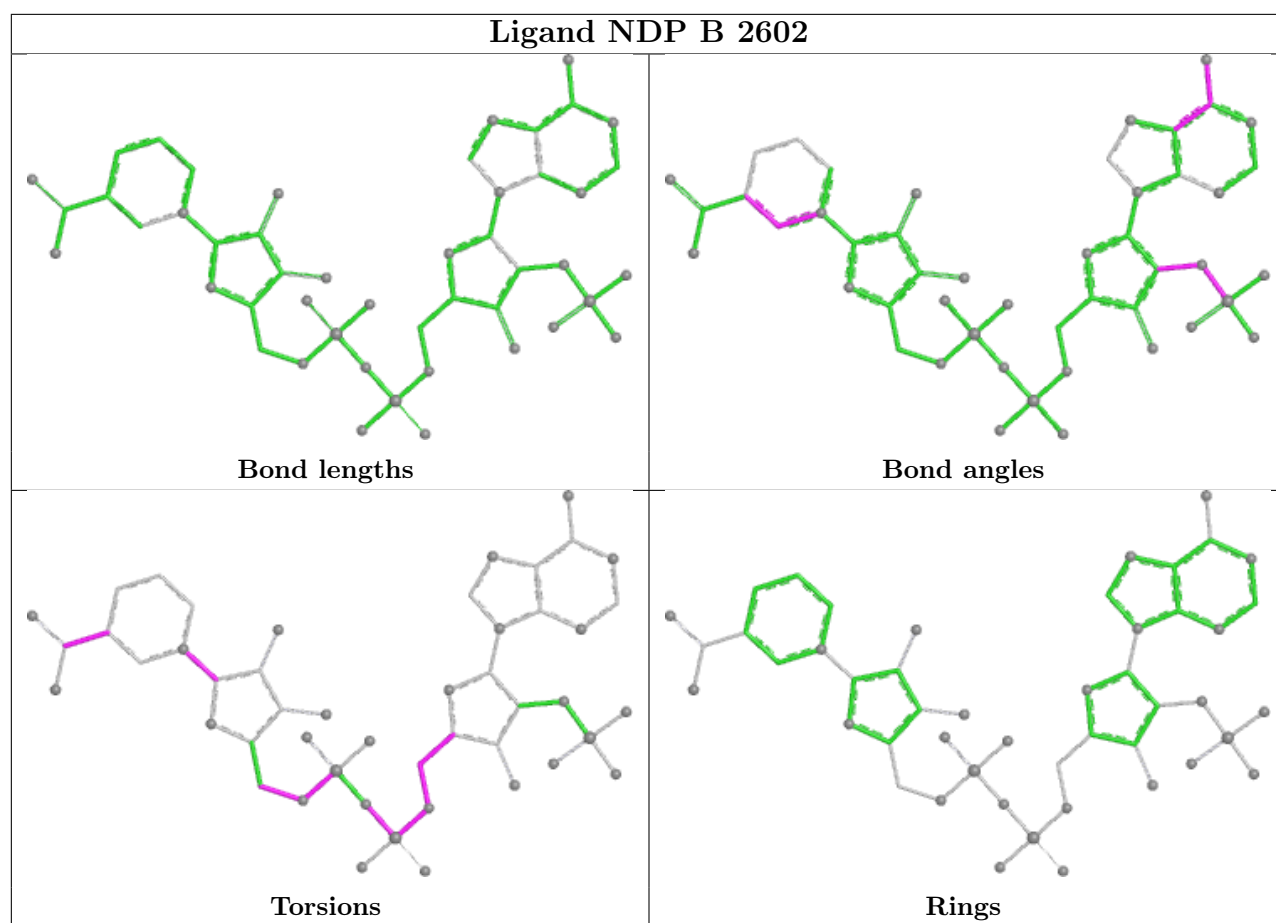
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-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 ⓘ
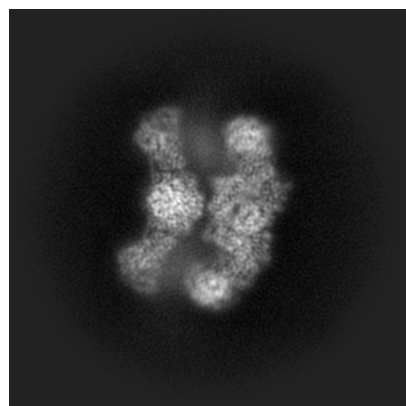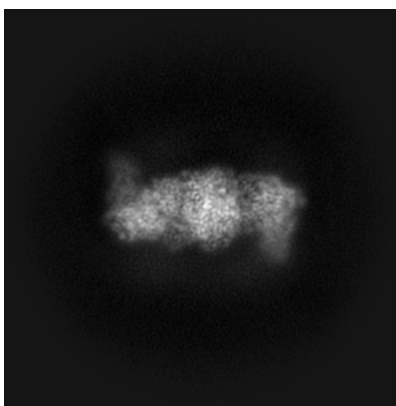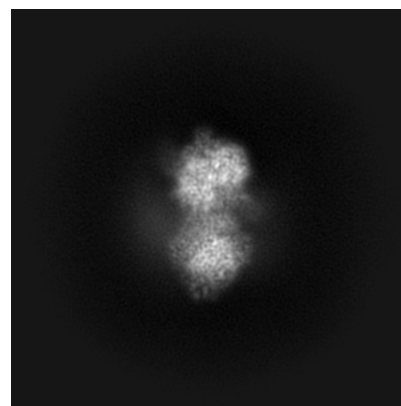
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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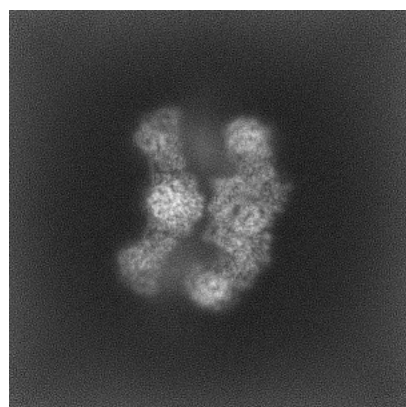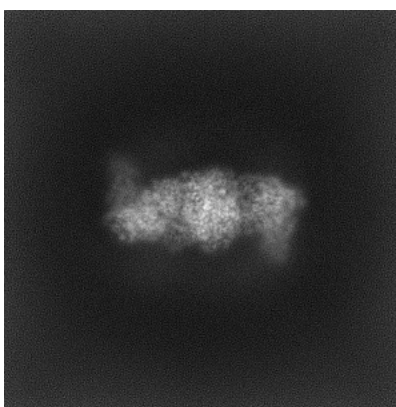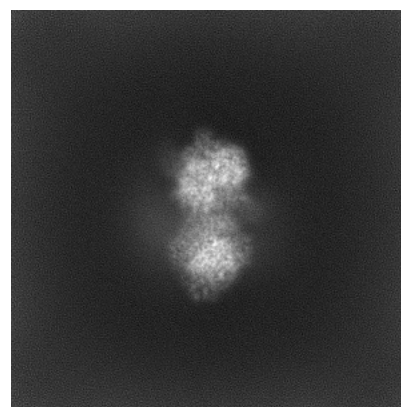
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
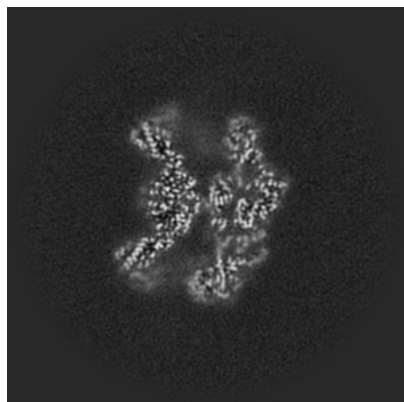
6.2.1 Primary map

X Index: 180
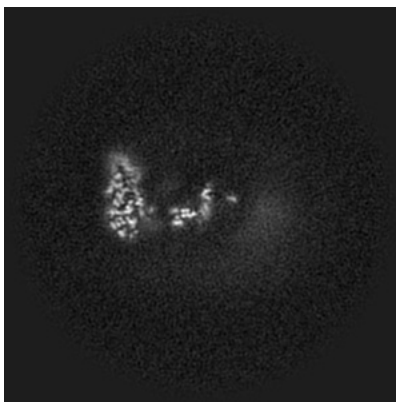
Y Index: 180
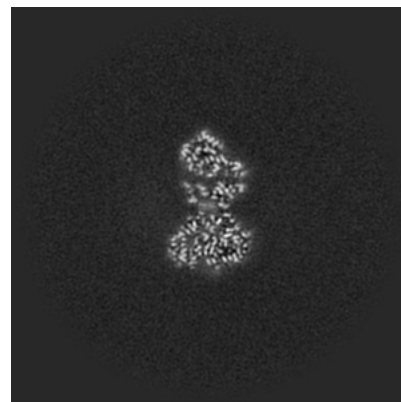
Z Index: 180

6.2.2 Raw map
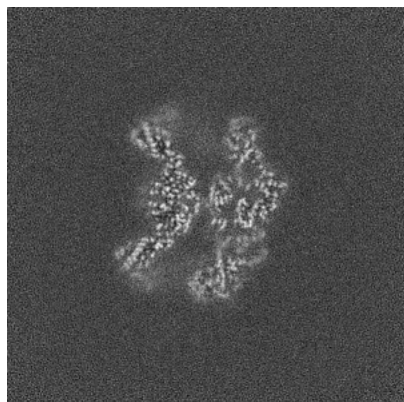
X Index: 180
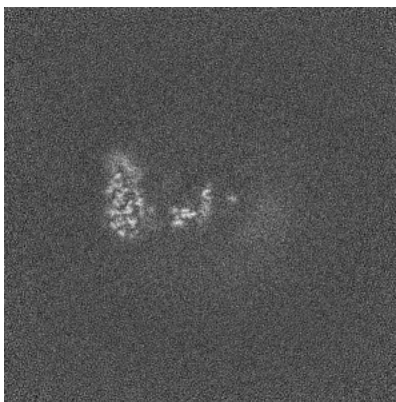
Y Index: 180
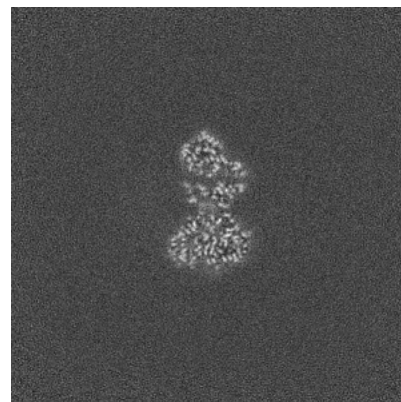
Z Index: 180

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

6.3 Largest variance slices (i)

6.3.1 Primary map
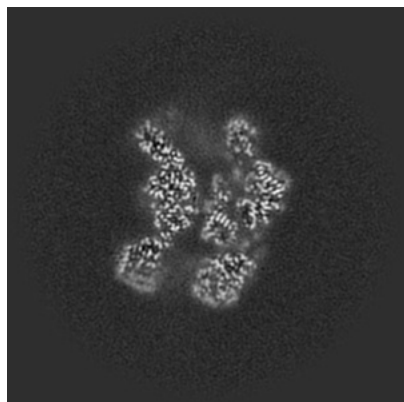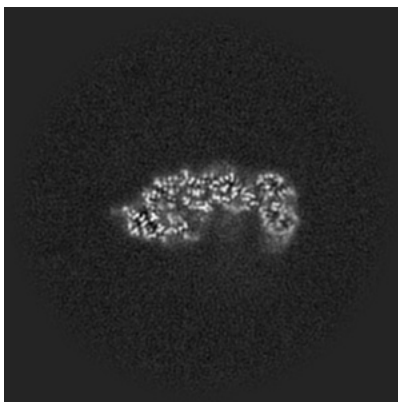
| X Index: 176 | Y Index: 208 | Z Index: 182 |
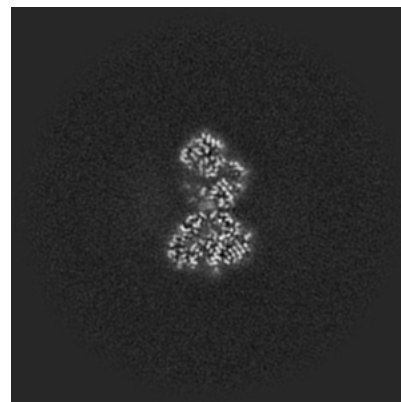
6.3.2 Raw map
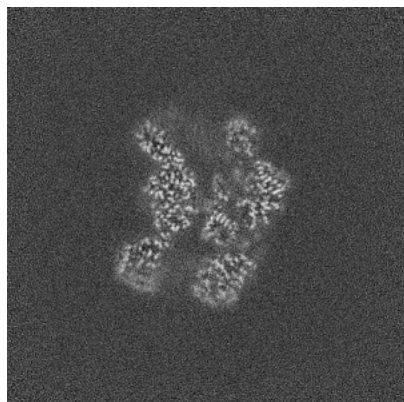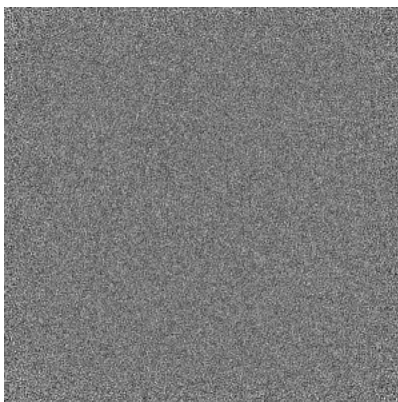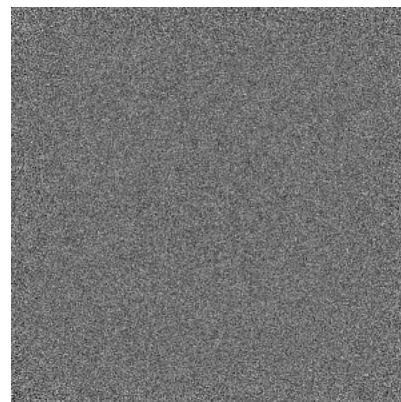
| X Index: 176 | Y Index: 0 | Z Index: 359 |

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

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

6.4.1 Primary map
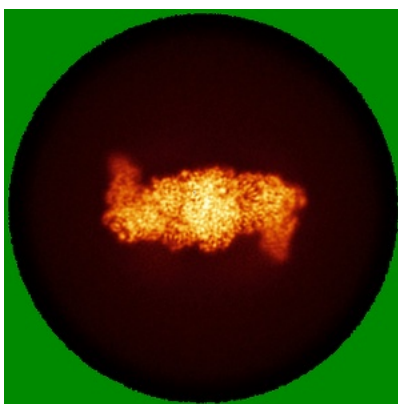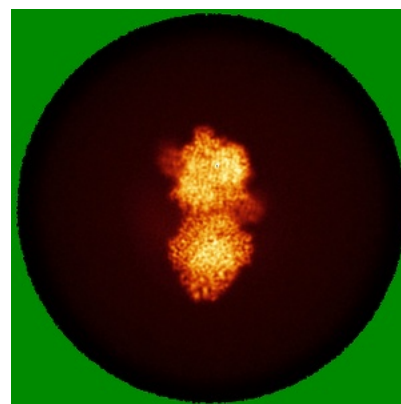
| X | Y | Z |

6.4.2 Raw map

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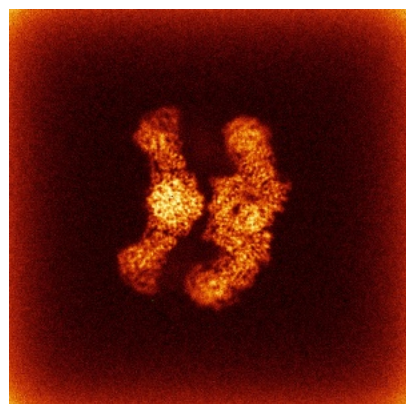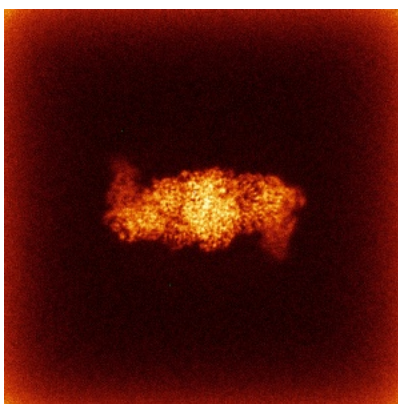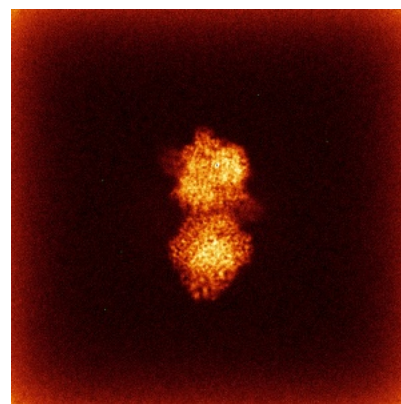
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ
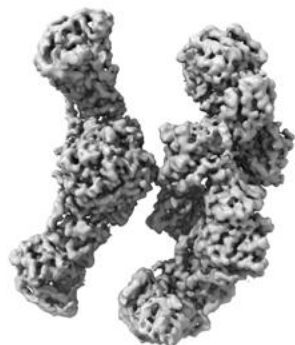
6.5.1 Primary map

X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.171. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map
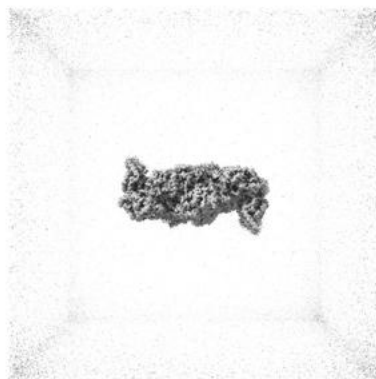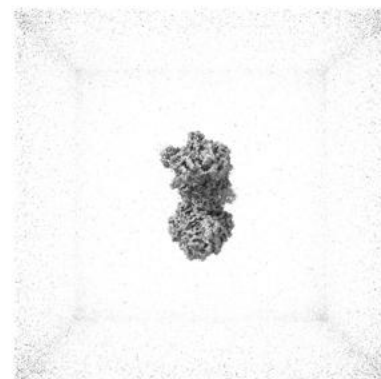
X	Y	Z

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

6.6 Mask visualisation (i)

This section 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
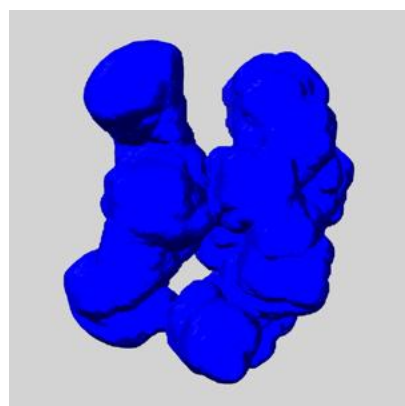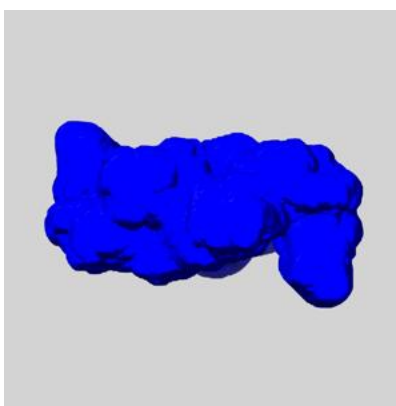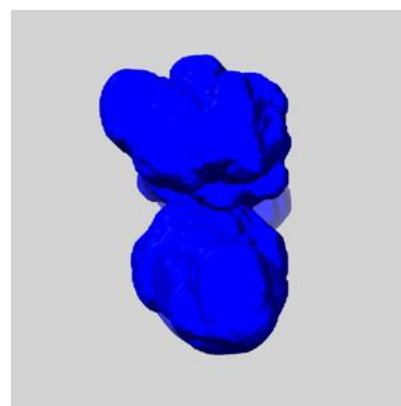
7 Map analysis ⓘ

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

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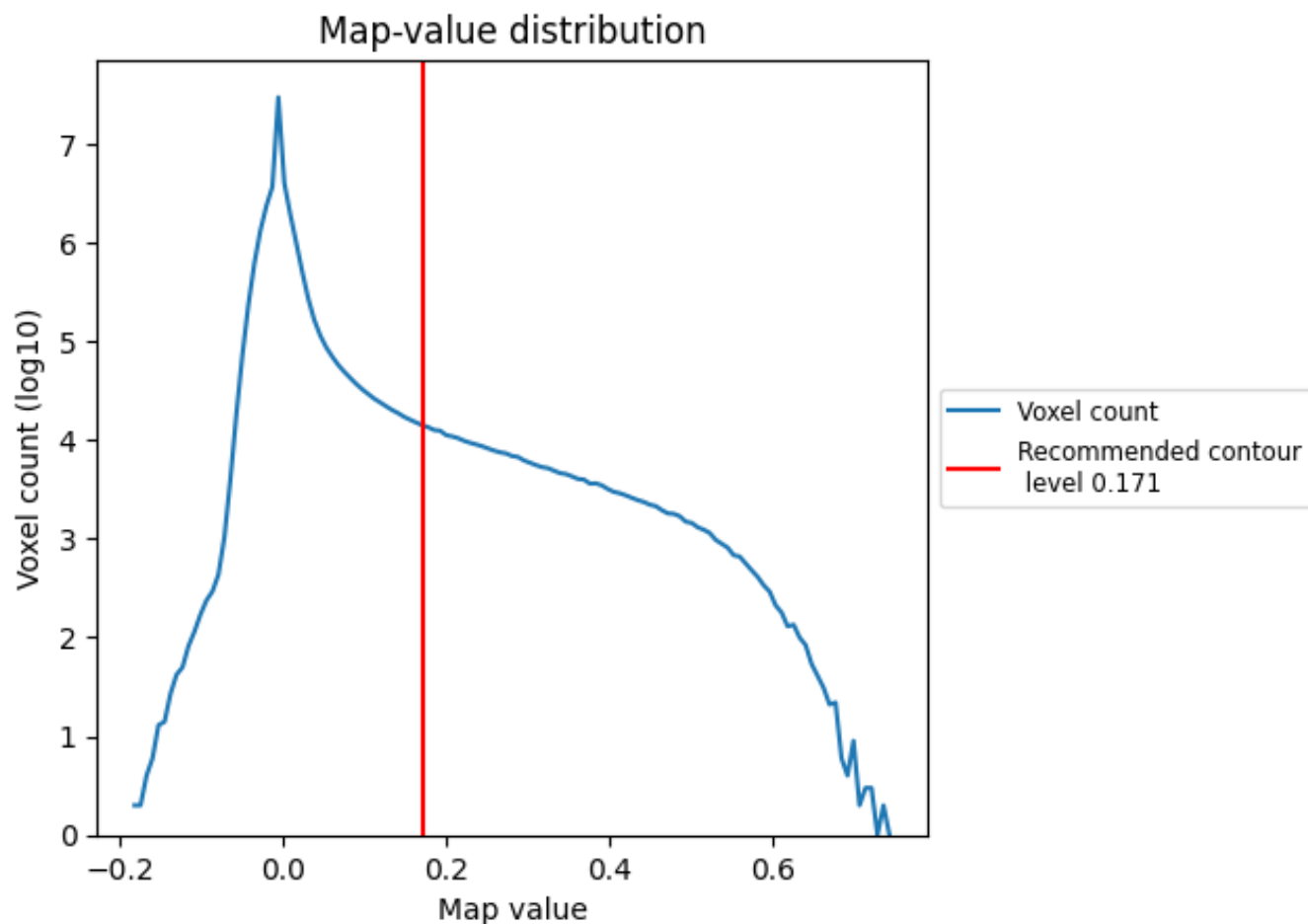
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
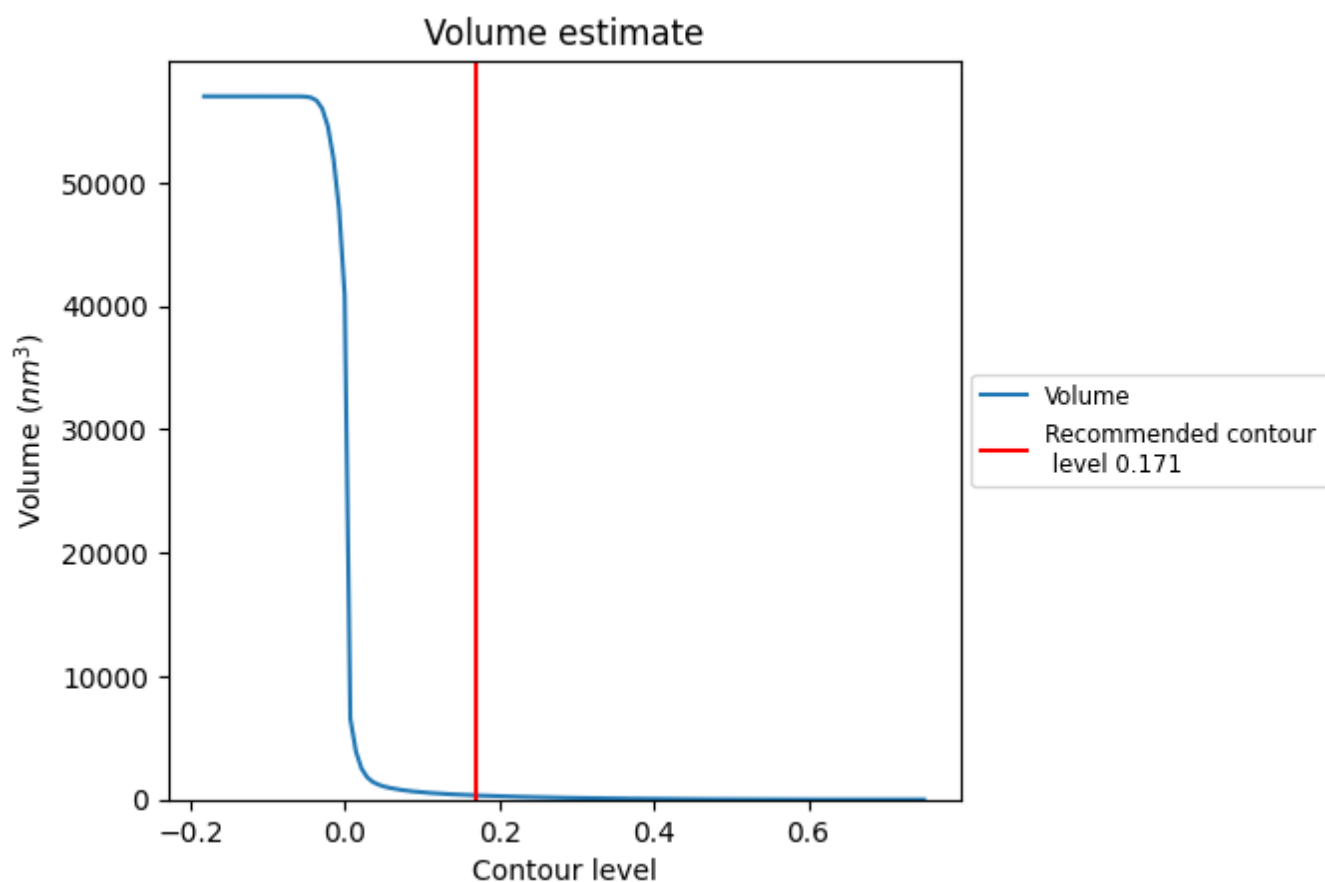
The volume at the recommended contour level is 336 nm^3; this corresponds to an approximate mass of 304 kDa.

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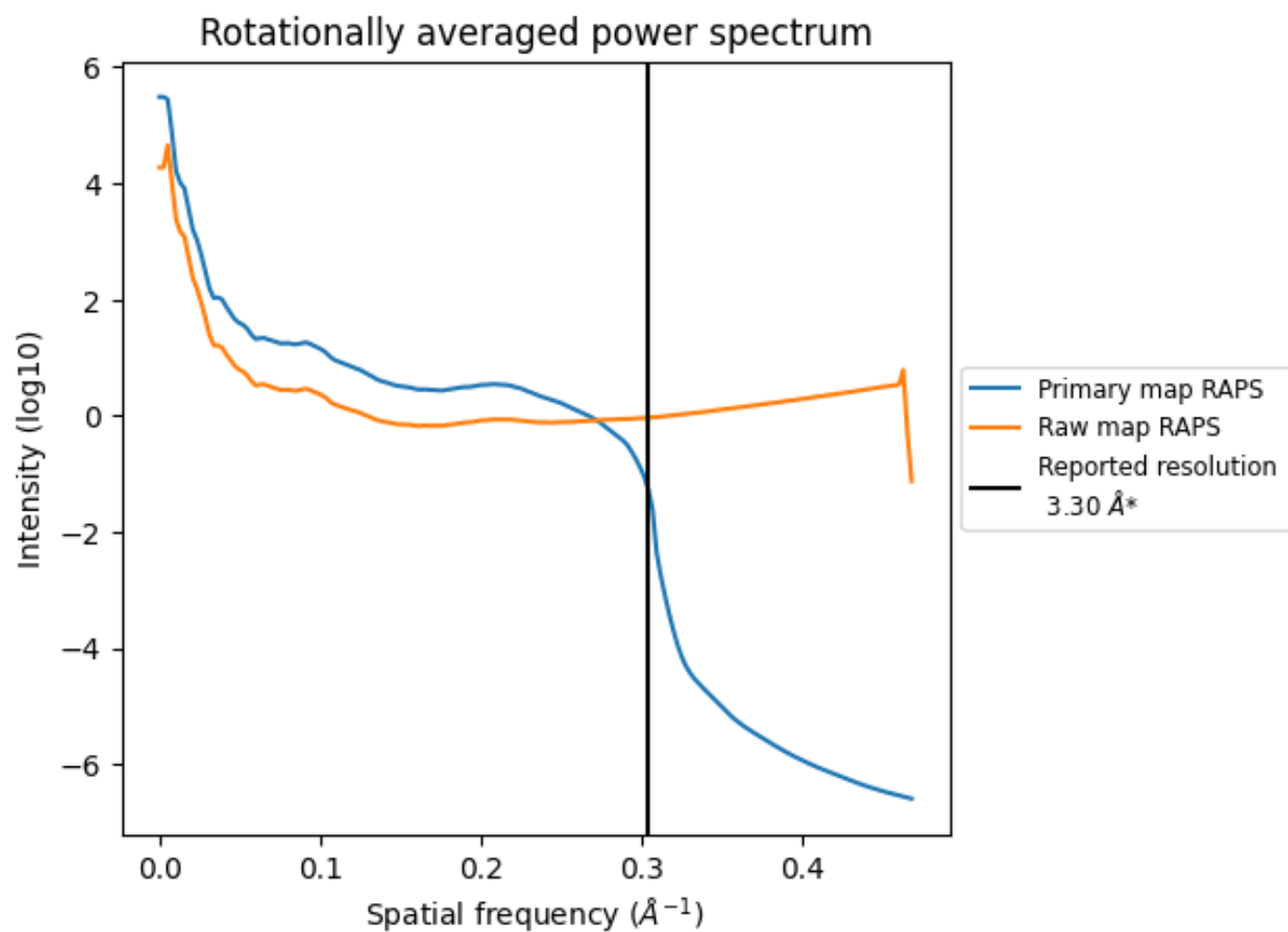
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8　Fourier-Shell correlation (i)

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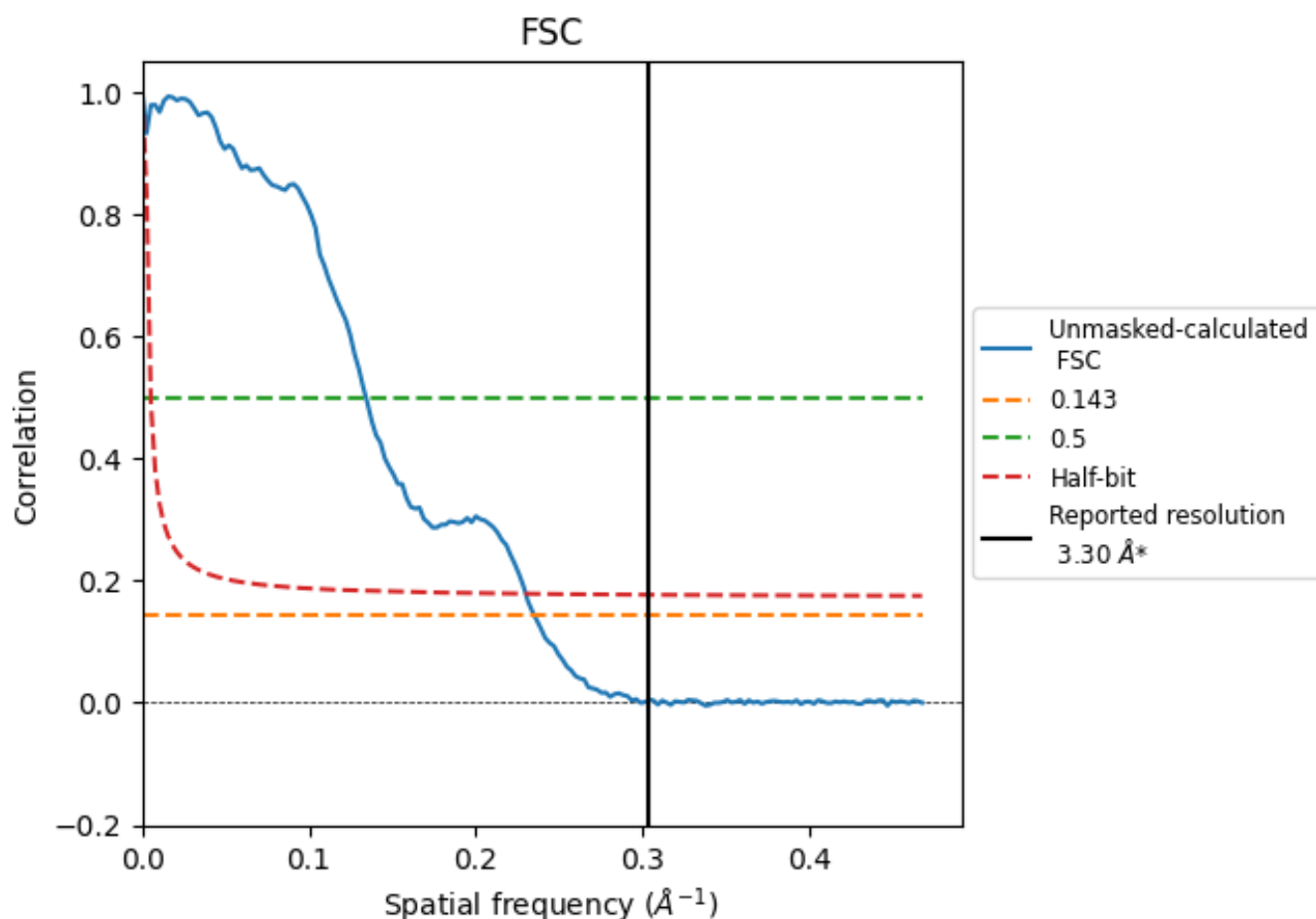
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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.
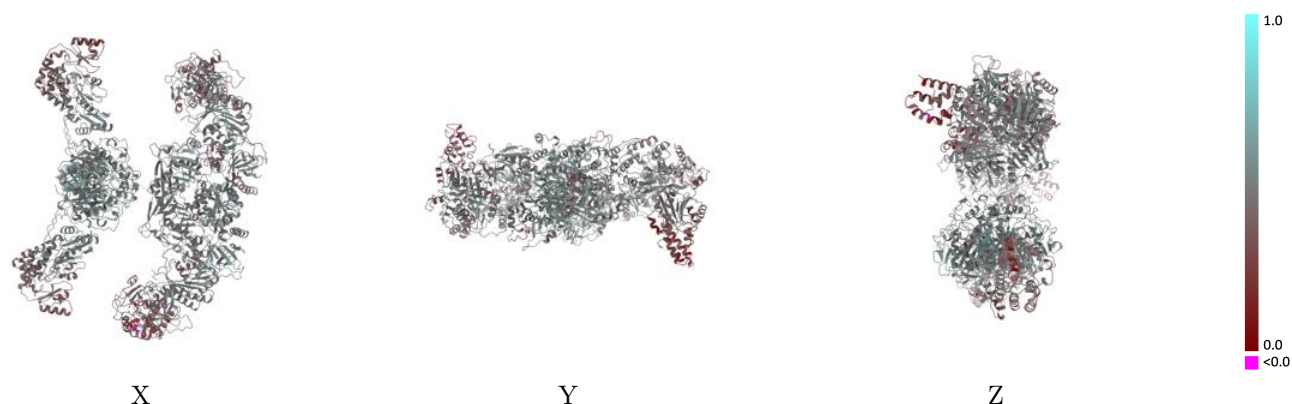
9.1 Map-model overlay ⓘ
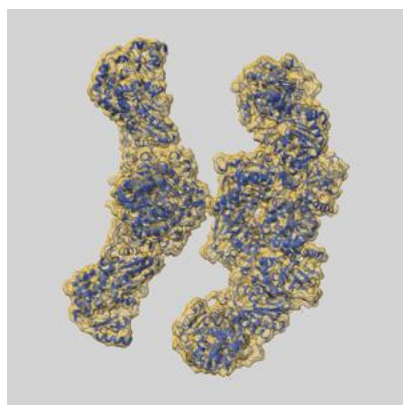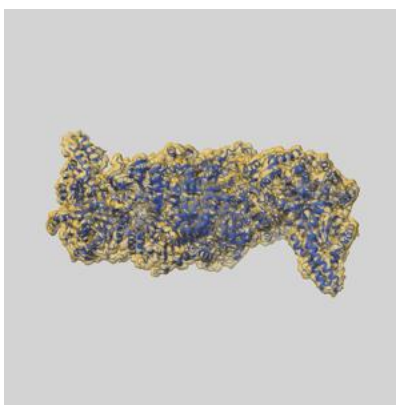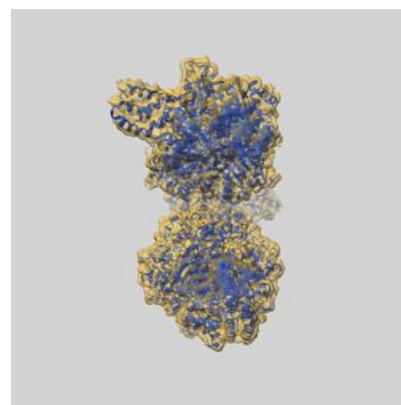
| X | Y | Z |

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 ⓘ

X   Y   Z

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

9.3   Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
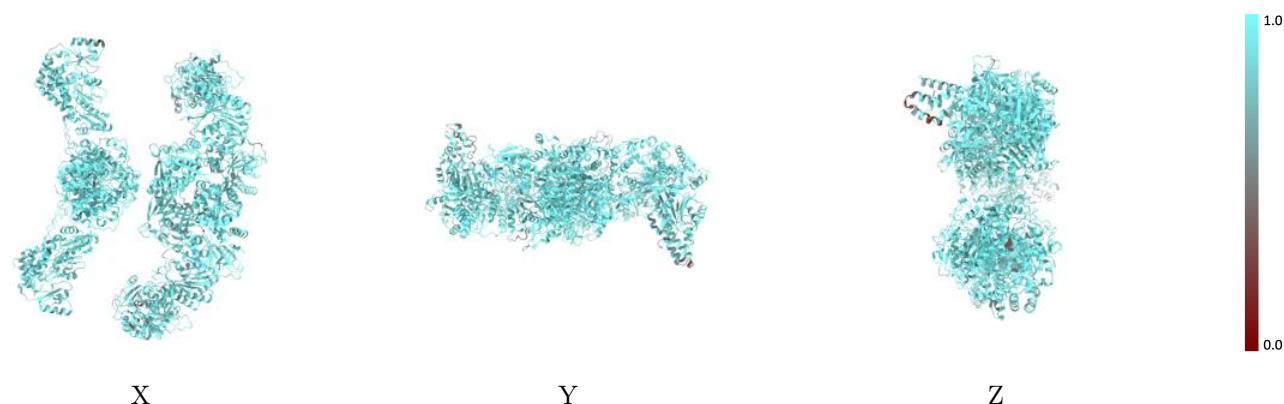
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.171).

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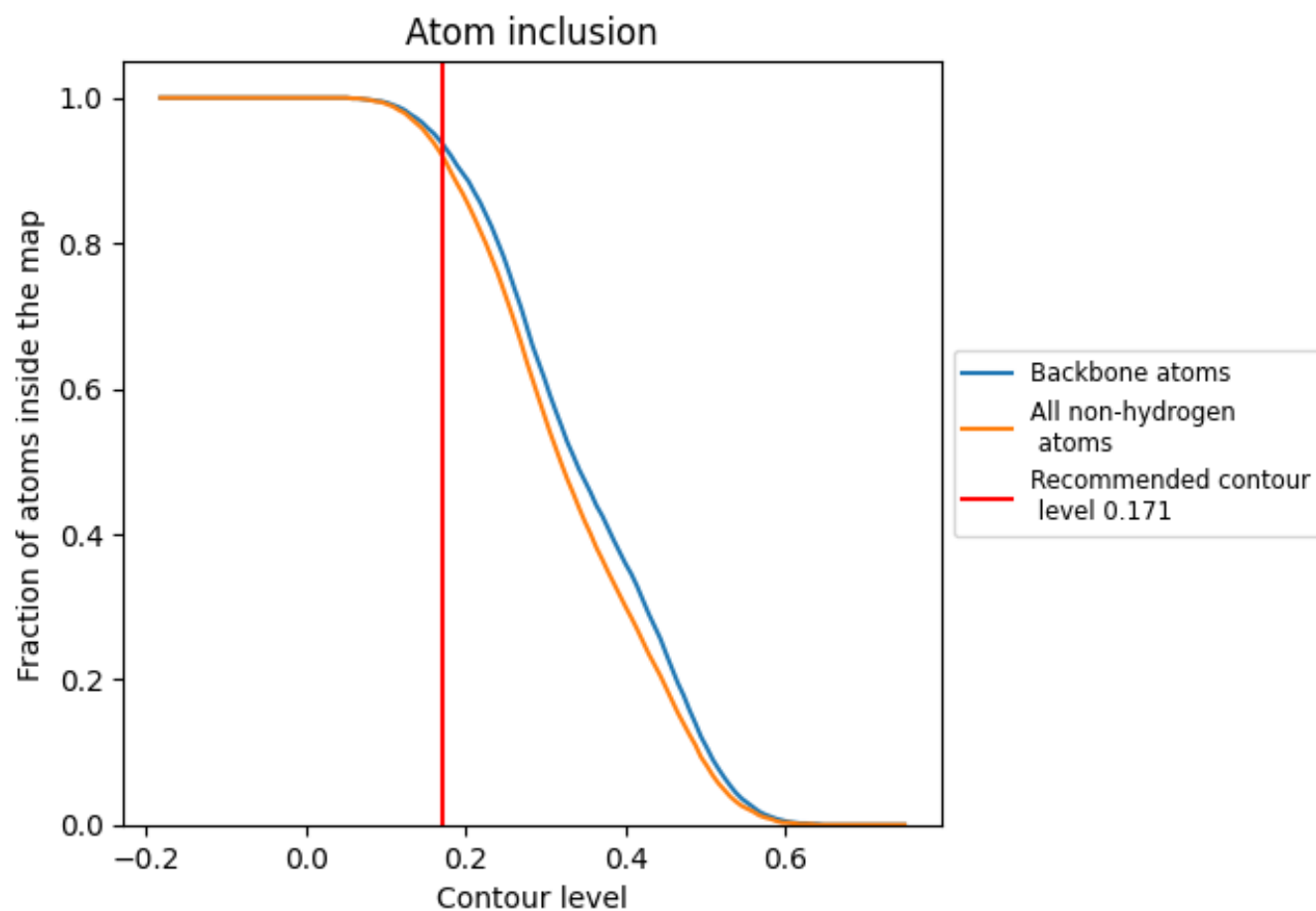
At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

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

1.0

0.0

<0.0