Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 11:22 AM JST

PDB ID	:	7YG5
EMDB ID	:	EMD-33808
Title	:	Structure of human R-type voltage-gated CaV2.3-alpha2/delta1-beta1 channel complex in the topiramate-bound state
Authors	:	Gao, Y.; Zhao, Y.
Deposited on	:	2022-07-11
Resolution	:	3.00 Å(reported)
Based on initial model	:	7VFS

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:

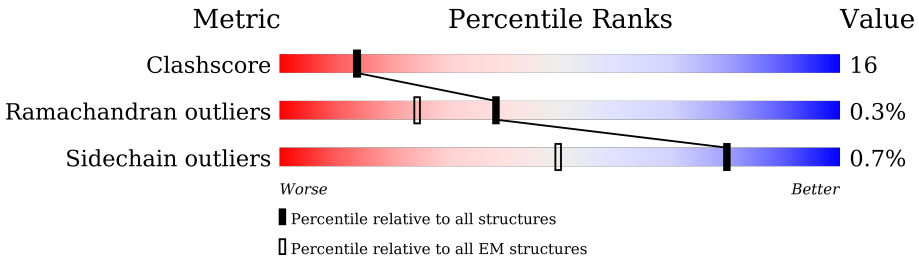
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.00 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	2313	9% 39% 17% · 43%
2	B	598	22% 16% 11% 73%
3	D	1103	14% 59% 28% 13%
4	C	3	33% 33% 33%
4	E	3	33% 33% 67%
5	F	3	67% 33% 33% 33%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 20308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Voltage-dependent R-type calcium channel subunit alpha-1E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1319	10674	7007	1761	1830	76	0	0

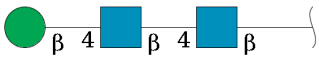
- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	162	1269	813	217	234	5	0	0

- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

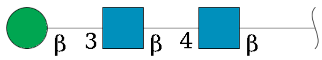
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	955	7637	4842	1281	1483	31	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



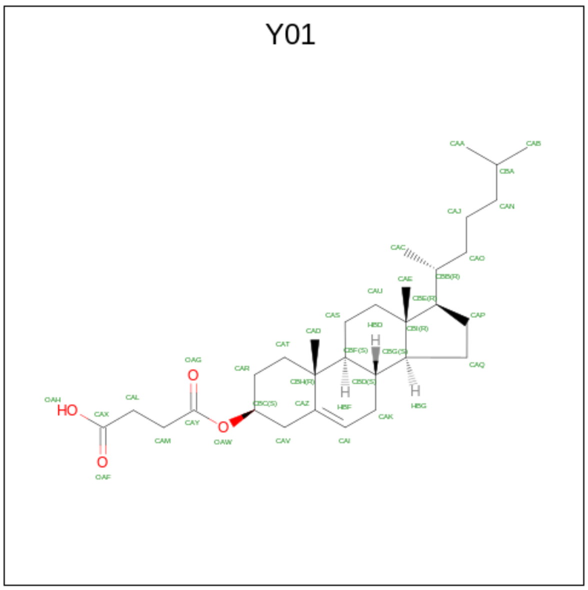
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	3	39	22	2	15	0	0
4	C	3	39	22	2	15	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	3	39	22	2	15	0	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0
6	A	1	Total 35	C 31	O 4	0

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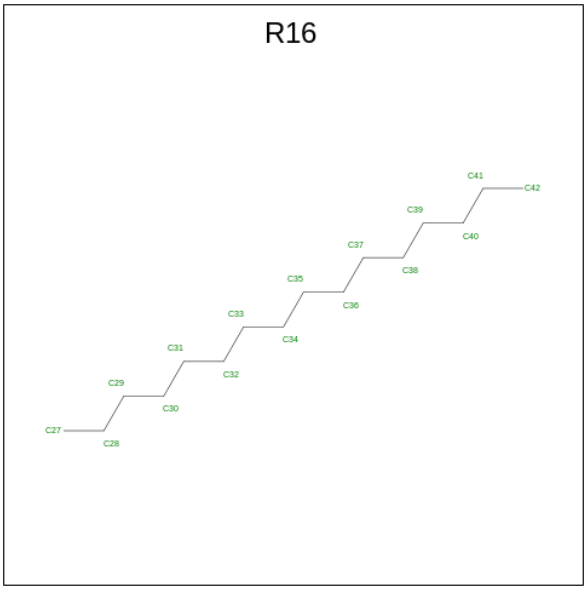
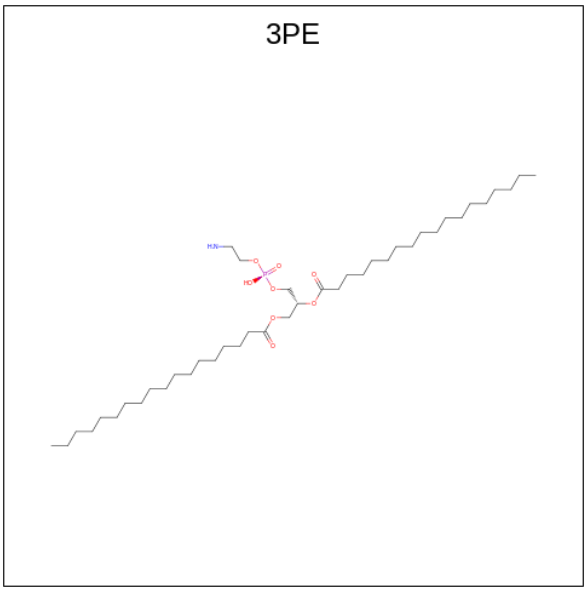
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 35 31 4	0

- Molecule 7 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 10 10	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 13 13	0
7	A	1	Total C 9 9	0
7	A	1	Total C 16 16	0

- Molecule 8 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).

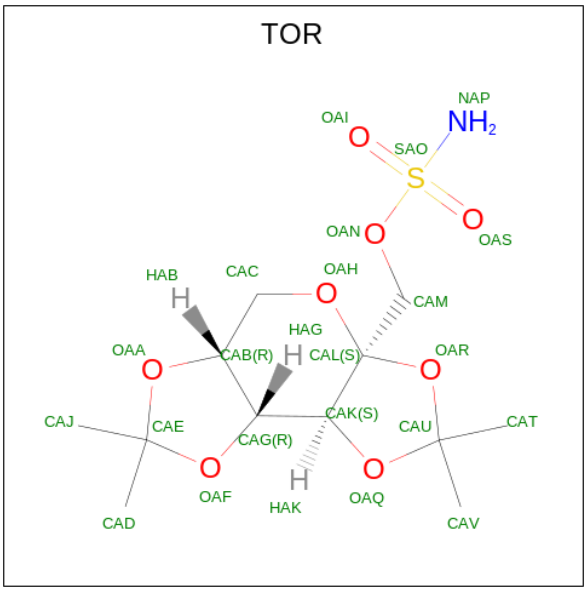


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

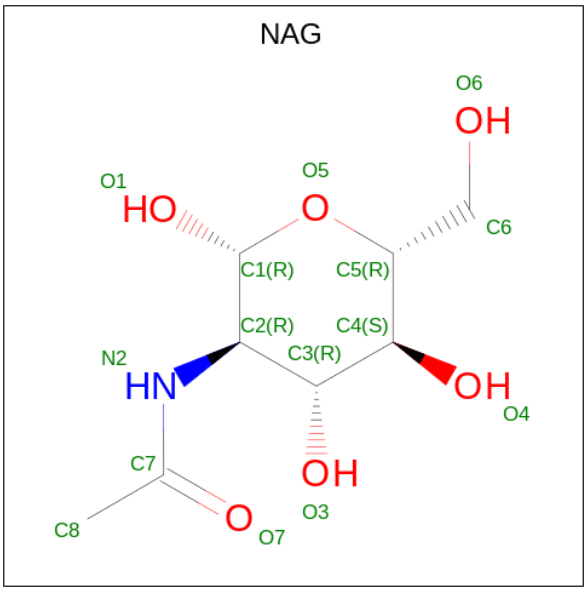
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Ca	0
			1	1	
9	D	1	Total	Ca	0
			1	1	

- Molecule 10 is [(3aS,5aR,8aR,8bS)-2,2,7,7-tetramethyltetrahydro-3aH-bis[1,3]dioxolo[4,5-b:4',5'-d]pyran-3a-yl]methyl sulfamate (three-letter code: TOR) (formula: $C_{12}H_{21}NO_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	S	0
			22	12	1	8	1	

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	

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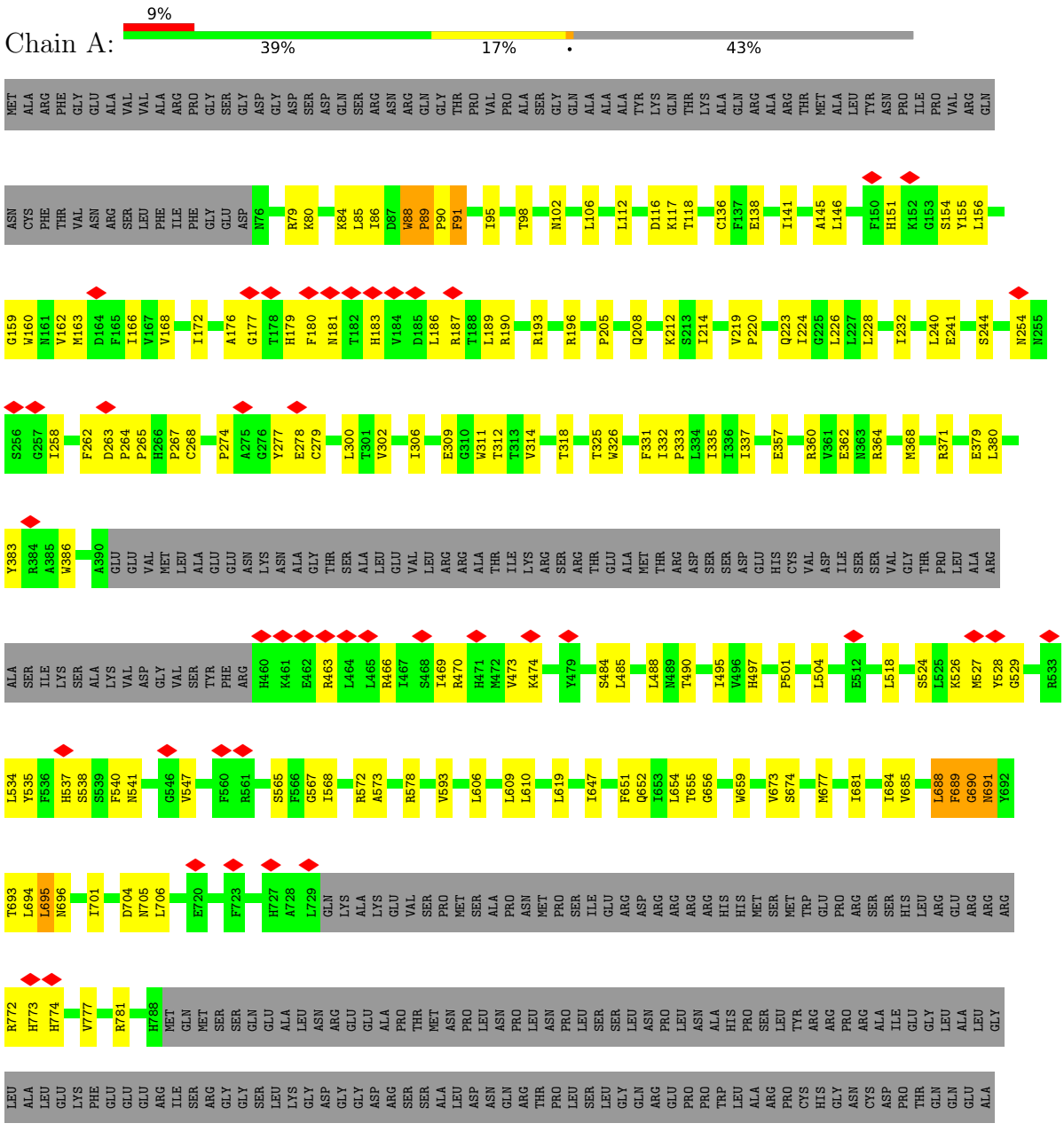
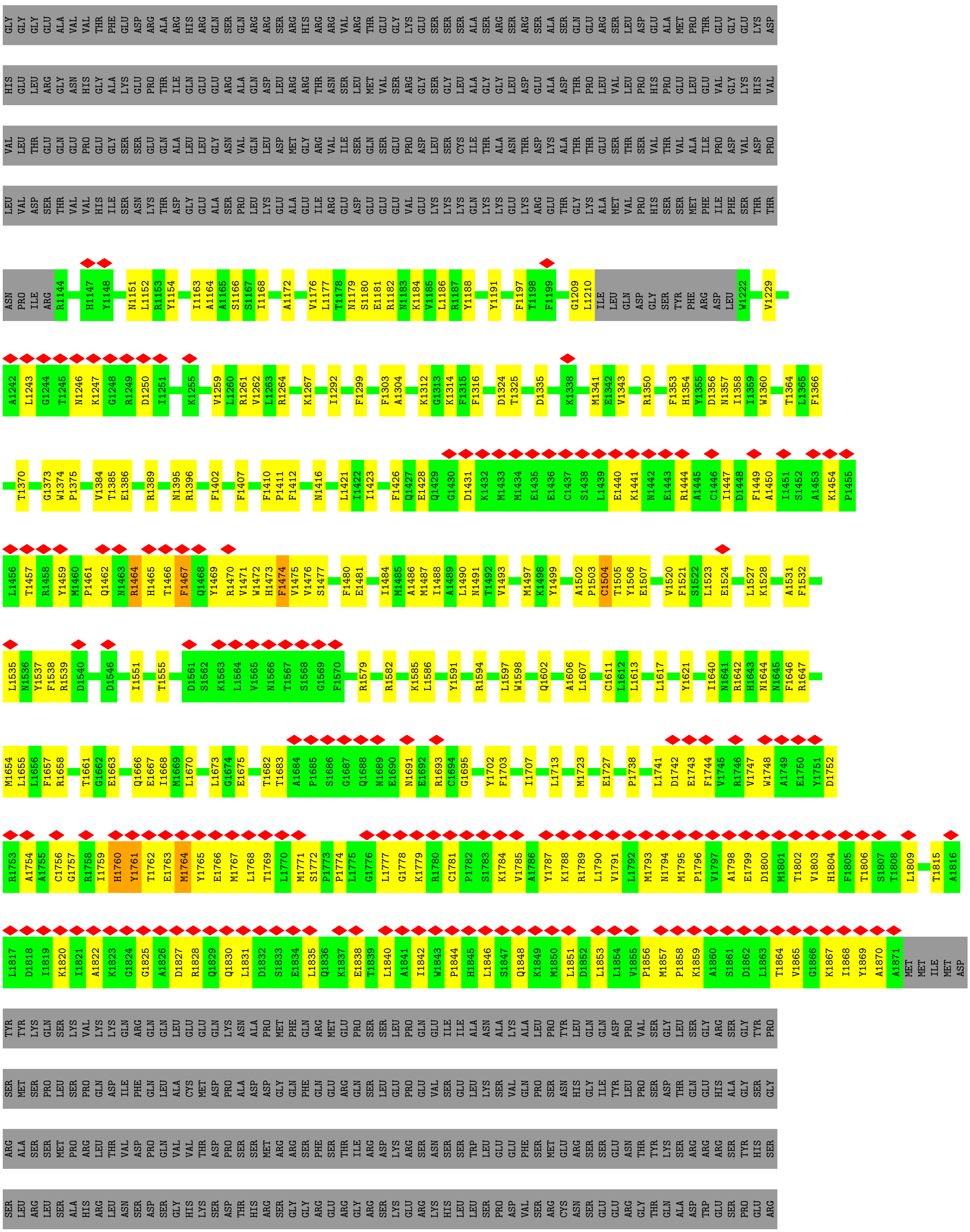
Mol	Chain	Residues	Atoms				AltConf
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	
11	D	1	Total	C	N	O	0
			14	8	1	5	

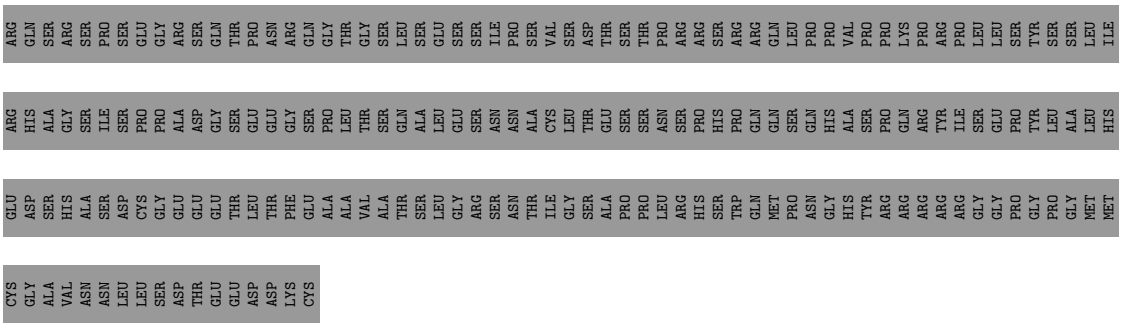
3 Residue-property plots (i)

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: Voltage-dependent R-type calcium channel subunit alpha-1E

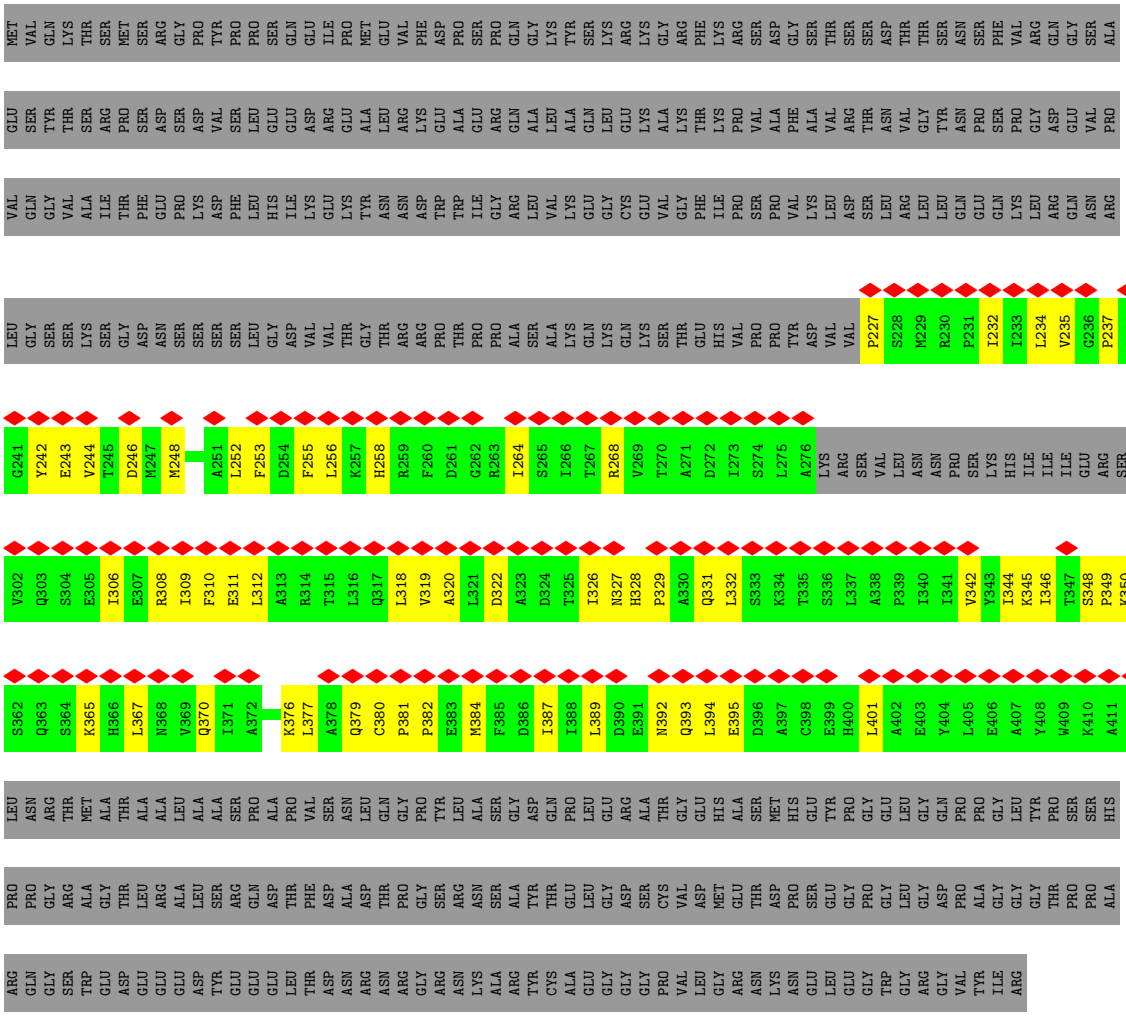



GLY GLY GLY GLU ALA VAL VAL THR PHE GLU ASP ARG ALA ARG HIS ARG GLN SER GLN ARG ARG SER ARG HIS ARG ARG VAL ARG THR GLU GLY LYS GLU SER SER SER ALA SER ARG SER ARG SER ALA SER GLN GLU ARG SER LEU ASP GLU ALA MET PRO THR GLU GLY GLU LYS ASP
HIS GLU LEU ARG GLY ASN HIS GLY ALA LYS GLU PRO THR ILE GLN GLU GLU ARG ALA GLN ASP LEU ARG ARG THR ASN SER LEU MET VAL SER ARG GLY SER GLY LEU ALA GLY GLY LEU ASP GLU ALA ASP THR PRO LEU VAL LEU PRO HIS PRO GLU LEU GLU VAL GLY LYS HIS VAL
VAL LEU THR GLU GLN GLU PRO GLU GLY SER SER GLU GLN ALA LEU LEU GLY ASN VAL GLN LEU ASP MET GLY ARG VAL ILE SER GLN SER GLU PRO ASP LEU SER CYS ILE THR ALA ASN THR ASP LYS ALA THR THR GLU SER THR SER VAL THR VAL ALA ILE PRO ASP VAL ASP PRO
LEU VAL ASP SER THR VAL VAL HIS ILE SER ASN LYS THR ASP GLY GLU ALA SER PRO LEU LYS GLU ALA GLU ILE ARG GLU ASP GLU GLU GLU VAL GLU LYS LYS GLN LYS LYS GLU LYS ARG GLU THR GLY LYS ALA MET VAL PRO HIS SER SER MET PHE ILE PHE SER THR THR
ASN PRO ILE ARG R1144 H1147 Y1148 N1151 L1152 R1153 Y1154 I1163 A1164 A1165 S1166 S1167 I1168 A1172 V1176 L1177 T1178 N1179 S1180 E1181 R1182 N1183 K1184 V1185 L1186 R1187 Y1188 Y1191 F1197 T1198 F1199 G1209 L1210 ILE LEU GLN ASP GLY SER TYR PHE ARG ASP LEU W1222 V1229
A1242 L1243 G1244 T1245 N1246 K1247 G1248 R1249 D1250 I1251 K1255 V1259 L1260 R1261 V1262 L1263 R1264 K1267 I1292 F1299 F1303 A1304 K1312 G1313 K1314 F1315 F1316 D1324 T1325 D1335 K1338 M1341 E1342 V1343 R1350 F1353 H1354 Y1355 D1356 N1357 I1358 I1359 W1360 T1364 L1365 F1366
T1370 G1373 W1374 P1375 V1384 T1385 E1386 R1389 N1395 R1396 F1402 F1407 F1410 P1411 F1412 N1416 L1421 I1422 I1423 F1426 Q1427 E1428 Q1429 G1430 D1431 K1432 M1433 M1434 E1435 E1436 C1437 S1438 L1439 E1440 K1441 N1442 E1443 R1444 A1445 C1446 I1447 D1448 F1449 A1450 I1451 S1452 A1453 K1454 P1455
L1456 T1457 R1458 Y1459 M1460 P1461 Q1462 N1463 R1464 H1465 T1466 F1467 Q1468 Y1469 R1470 V1471 W1472 H1473 F1474 V1475 V1476 S1477 F1480 E1481 I1484 M1485 A1486 M1487 I1488 A1489 L1490 N1491 T1492 V1493 M1497 K1498 Y1499 A1502 P1503 C1504 T1505 Y1506 E1507 V1520 F1521 S1522 L1523 E1524 L1527 K1528 A1531 F1532
L1535 N1536 Y1537 F1538 R1539 D1540 D1546 I1551 T1555 D1561 S1562 K1563 L1564 V1565 N1566 T1567 S1568 G1569 F1570 R1579 R1582 K1585 L1586 Y1591 R1594 L1597 W1598 Q1602 A1606 L1607 C1611 L1612 L1613 L1617 Y1621 I1640 N1641 R1642 H1643 N1644 N1645 F1646 R1647
M1654 L1655 L1656 F1657 R1658 T1661 G1662 E1663 Q1666 E1667 I1668 M1669 L1670 L1673 G1674 E1675 T1682 T1683 A1684 P1685 S1686 G1687 Q1688 N1689 E1690 N1691 E1692 R1693 C1694 G1695 Y1702 F1703 I1707 L1713 M1723 E1727 P1738 L1741 D1742 E1743 F1744 V1745 R1746 V1747 W1748 A1749 E1750 Y1751 D1752
R1753 A1754 A1755 C1756 G1757 R1758 I1759 H1760 Y1761 T1762 E1763 M1764 Y1765 E1766 M1767 L1768 T1769 L1770 M1771 S1772 P1773 P1774 L1775 G1776 L1777 G1778 K1779 R1780 C1781 P1782 S1783 K1784 V1785 A1786 Y1787 K1788 R1789 L1790 V1791 L1792 M1793 N1794 M1795 P1796 V1797 A1798 E1799 D1800 M1801 T1802 V1803 H1804 F1805 T1806 S1807 T1808 L1809 T1815 A1816
L1817 D1818 I1819 K1820 I1821 A1822 K1823 G1824 G1825 A1826 D1827 R1828 Q1829 Q1830 L1831 D1832 S1833 E1834 L1835 Q1836 K1837 E1838 T1839 L1840 A1841 I1842 W1843 P1844 H1845 L1846 S1847 Q1848 K1849 M1850 L1851 D1852 L1853 L1854 V1855 P1856 M1857 P1858 K1859 A1860 S1861 D1862 L1863 T1864 V1865 G1866 K1867 I1868 Y1869 A1870 A1871 MET MET ILE MET ASP
TYR TYR LYS GLN SER LYS VAL LYS LYS GLN ARG GLN GLN LEU GLU GLU GLN LYS ASN ALA PRO MET PHE GLN ARG MET GLU PRO SER SER LEU PRO GLN GLU ILE ILE ALA ASN ALA LYS ALA LEU PRO TYR LEU GLN GLN ASP PRO VAL SER GLY LEU SER GLY ARG SER GLY TYR PRO
SER MET SER PRO LEU SER PRO GLN ASP ILE PHE GLN LEU ALA CYS MET ASP PRO ALA ASP ASP GLY GLY PHE GLN GLU ARG GLN SER LEU GLU PRO GLU VAL SER GLU LEU LYS SER VAL GLN PRO SER ASN HIS GLY ILE TYR LEU PRO SER ASP THR GLN GLU HIS ALA GLY SER GLY
ARG ALA SER SER MET PRO ARG LEU THR VAL ASP PRO GLN VAL VAL THR ASP PRO SER SER MET ARG ARG SER PHE SER THR ILE ARG ASP LYS ARG SER ASN SER SER TRP LEU GLU GLU PHE SER MET GLU ARG SER SER GLU ASN THR TYR LYS SER ARG ARG ARG SER TYR HIS SER
SER LEU ARG LEU SER ALA HIS ARG LEU ASN SER ASP SER GLY HIS LYS SER ASP THR HIS ARG SER GLY GLY ARG GLU ARG GLY ARG SER LYS GLU ARG LYS HIS LEU LEU SER PRO ASP VAL SER ARG CYS ASN SER GLU GLU ARG GLY THR GLN ALA ASP TRP GLU SER PRO GLU ARG



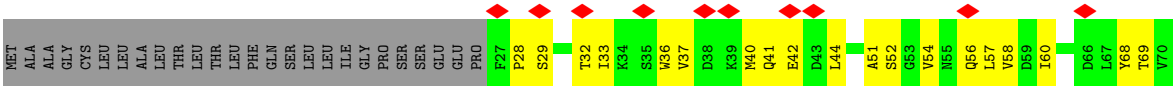
• Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

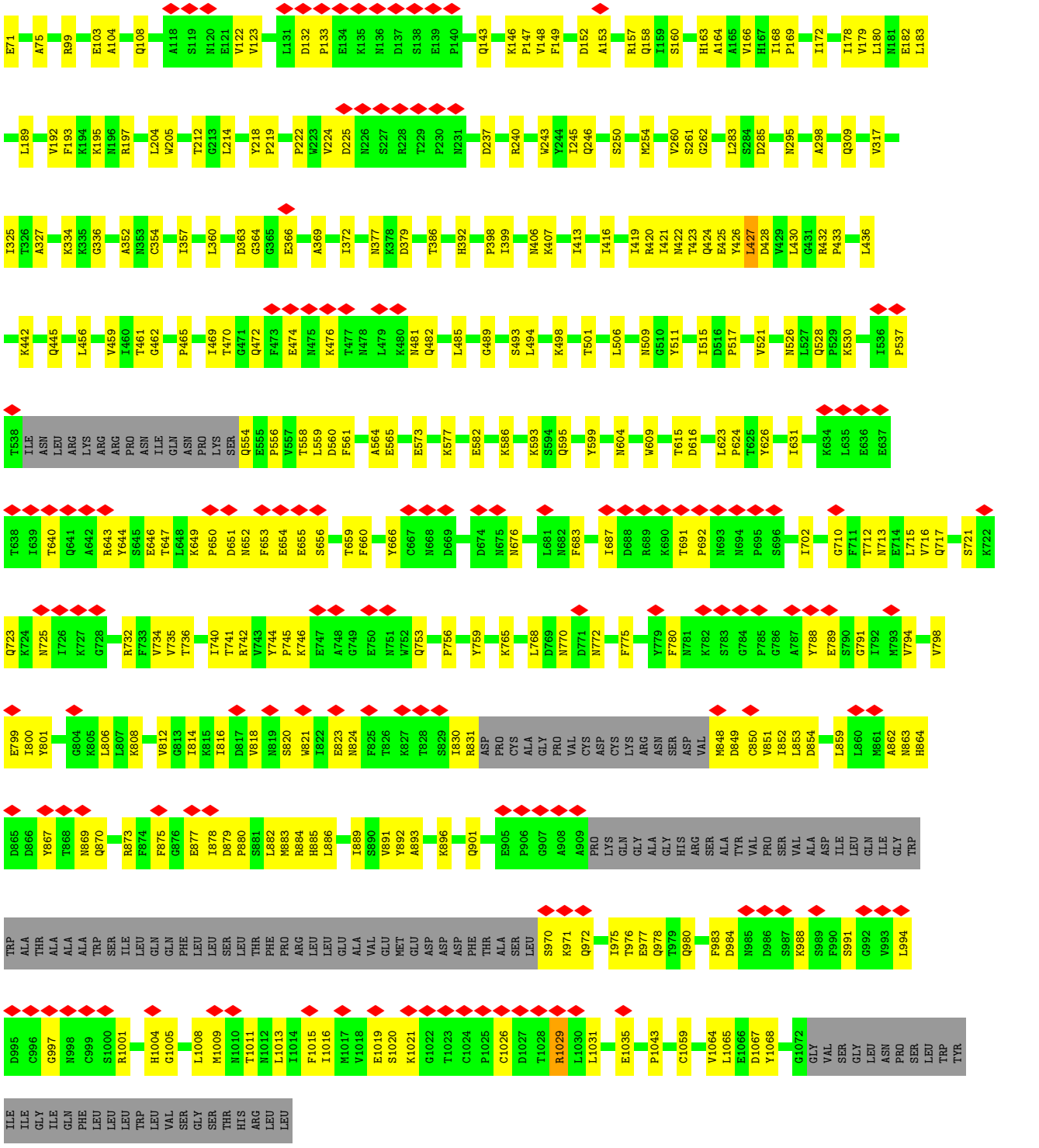
Chain B:



• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:



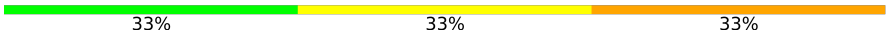


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

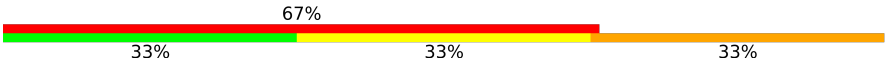
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 5: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	135000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.883	Depositor
Minimum map value	-2.363	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TOR, R16, NAG, BMA, 3PE, CA, Y01

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	0.68	2/10939 (0.0%)	0.62	3/14805 (0.0%)
2	B	0.31	0/1290	0.51	0/1744
3	D	0.66	0/7799	0.59	1/10578 (0.0%)
All	All	0.65	2/20028 (0.0%)	0.60	4/27127 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	CYS	CB-SG	-6.26	1.71	1.82
1	A	268	CYS	CB-SG	-5.39	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1356	ASP	CB-CA-C	-5.74	98.92	110.40
1	A	706	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	268	CYS	CA-CB-SG	5.61	124.09	114.00
3	D	427	LEU	CB-CG-CD1	-5.43	101.77	111.00

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	10674	0	10813	342	0
2	B	1269	0	1290	57	0
3	D	7637	0	7426	225	0
4	C	39	0	34	4	0
4	E	39	0	34	0	0
5	F	39	0	34	2	0
6	A	315	0	441	34	0
7	A	80	0	163	3	0
8	A	80	0	108	0	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	22	0	18	5	0
11	D	112	0	104	2	0
All	All	20308	0	20465	631	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 (631) 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:1466:THR:HB	1:A:1470:ARG:NH2	1.63	1.12
10:A:2416:TOR:OAA	10:A:2416:TOR:CAB	1.64	1.11
1:A:1759:ILE:HG13	1:A:1763:GLU:HB2	1.32	1.06
1:A:89:PRO:HB2	1:A:90:PRO:HD3	1.35	1.01
1:A:1466:THR:HB	1:A:1470:ARG:HH21	1.27	0.98
1:A:1467:PHE:HA	1:A:1470:ARG:HB3	1.55	0.87
3:D:1001:ARG:HD3	3:D:1020:SER:HB3	1.58	0.84
3:D:650:PRO:HA	3:D:653:PHE:HE2	1.42	0.84
3:D:650:PRO:HA	3:D:653:PHE:CE2	2.13	0.83
2:B:235:VAL:HG23	2:B:240:LYS:HZ1	1.45	0.82
2:B:312:LEU:HB3	2:B:319:VAL:HG21	1.59	0.82
10:A:2416:TOR:OAA	10:A:2416:TOR:CAC	2.26	0.81
3:D:875:PHE:HB3	3:D:883:MET:HE1	1.63	0.79
1:A:88:TRP:CD1	1:A:90:PRO:HD2	2.17	0.79
1:A:1247:LYS:HB3	1:A:1250:ASP:OD2	1.83	0.79
1:A:88:TRP:NE1	1:A:90:PRO:HD2	1.98	0.79
2:B:232:ILE:HB	2:B:320:ALA:HA	1.63	0.79
2:B:328:HIS:HB2	2:B:331:GLN:HB2	1.63	0.79
1:A:540:PHE:HB2	1:A:578:ARG:HH21	1.47	0.78
3:D:245:ILE:HG23	3:D:427:LEU:HD11	1.65	0.77
1:A:1795:MET:HE3	1:A:1803:VAL:HG11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:442:LYS:NZ	3:D:465:PRO:O	2.20	0.75
1:A:102:ASN:HD21	1:A:196:ARG:HH11	1.33	0.74
2:B:353:GLN:HB3	2:B:357:LYS:NZ	2.01	0.74
3:D:880:PRO:HB2	3:D:884:ARG:HH12	1.52	0.74
6:A:2417:Y01:HAC1	6:A:2417:Y01:HAE2	1.70	0.73
3:D:205:TRP:HE1	3:D:456:LEU:HD13	1.54	0.73
1:A:1505:THR:HG23	6:A:2401:Y01:HAI	1.69	0.73
1:A:1822:ALA:HB2	1:A:1831:LEU:HD12	1.71	0.72
1:A:1324:ASP:OD2	1:A:1389:ARG:NH2	2.22	0.72
3:D:377:ASN:ND2	3:D:406:ASN:OD1	2.24	0.71
3:D:994:LEU:HB3	3:D:1001:ARG:HB2	1.73	0.71
1:A:1762:THR:HA	1:A:1765:TYR:CE2	2.26	0.71
2:B:264:ILE:HG12	2:B:318:LEU:HB2	1.71	0.71
1:A:223:GLN:HE22	1:A:226:LEU:HD12	1.56	0.70
1:A:312:THR:HG21	1:A:1658:ARG:HG3	1.73	0.70
1:A:501:PRO:HD2	1:A:504:LEU:HD12	1.74	0.69
1:A:704:ASP:HB2	10:A:2416:TOR:HAJB	1.75	0.69
1:A:1464:ARG:HH21	1:A:1469:TYR:HB3	1.56	0.69
3:D:1005:GLY:HA3	3:D:1016:ILE:HD13	1.74	0.69
3:D:660:PHE:HB3	3:D:676:ASN:HD21	1.58	0.69
3:D:58:VAL:HG22	3:D:798:VAL:HG13	1.76	0.68
1:A:1804:HIS:CG	1:A:1853:LEU:HD11	2.29	0.68
1:A:1229:VAL:HG11	1:A:1267:LYS:HZ1	1.59	0.68
1:A:1598:TRP:NE1	1:A:1602:GLN:OE1	2.26	0.67
3:D:51:ALA:O	3:D:732:ARG:NH1	2.27	0.67
1:A:89:PRO:HB2	1:A:90:PRO:CD	2.17	0.67
2:B:244:VAL:HG21	2:B:356:ILE:HD13	1.76	0.67
1:A:1499:TYR:OH	1:A:1503:PRO:HD3	1.95	0.66
3:D:528:GLN:O	3:D:901:GLN:NE2	2.29	0.66
1:A:88:TRP:CE2	1:A:90:PRO:HD2	2.30	0.66
1:A:1586:LEU:HD13	6:A:2412:Y01:HAP2	1.77	0.66
1:A:79:ARG:HG3	1:A:80:LYS:H	1.58	0.66
3:D:666:TYR:HB3	3:D:702:ILE:HD11	1.77	0.66
1:A:1471:VAL:HG23	1:A:1472:TRP:H	1.61	0.66
3:D:660:PHE:HB3	3:D:676:ASN:ND2	2.10	0.66
1:A:88:TRP:HB2	1:A:89:PRO:HD2	1.76	0.66
1:A:1763:GLU:HA	1:A:1766:GLU:HB3	1.78	0.65
2:B:237:PRO:HD3	2:B:344:ILE:HB	1.77	0.65
3:D:29:SER:HB3	3:D:32:THR:HG23	1.77	0.65
2:B:232:ILE:HD11	2:B:318:LEU:HD12	1.79	0.65
1:A:155:TYR:HD2	1:A:156:LEU:HD22	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ARG:NH2	1:A:1727:GLU:OE1	2.31	0.64
1:A:1793:MET:HB3	1:A:1815:THR:HG21	1.77	0.64
2:B:240:LYS:NZ	2:B:326:ILE:O	2.25	0.64
3:D:517:PRO:HG2	3:D:616:ASP:HB2	1.80	0.64
1:A:1675:GLU:OE1	1:A:1693:ARG:NE	2.31	0.63
1:A:1441:LYS:HB2	1:A:1444:ARG:NH2	2.12	0.63
1:A:1407:PHE:HA	1:A:1411:PRO:HD2	1.79	0.63
1:A:1506:TYR:HD1	6:A:2401:Y01:HBD	1.62	0.63
6:A:2412:Y01:HAK1	6:A:2417:Y01:HAS2	1.81	0.63
3:D:157:ARG:NH2	3:D:222:PRO:O	2.31	0.63
1:A:241:GLU:OE2	1:A:1579:ARG:NH2	2.31	0.63
3:D:485:LEU:HD22	4:C:1:NAG:H82	1.81	0.63
1:A:1457:THR:HB	1:A:1459:TYR:CD2	2.34	0.63
1:A:1473:HIS:O	1:A:1474:PHE:C	2.36	0.63
3:D:260:VAL:HG11	3:D:325:ILE:HG12	1.80	0.63
3:D:240:ARG:HA	3:D:245:ILE:HD11	1.81	0.62
1:A:112:LEU:HD21	1:A:118:THR:HG23	1.81	0.62
1:A:1172:ALA:O	1:A:1182:ARG:NH1	2.32	0.62
1:A:1658:ARG:NH1	1:A:1663:GLU:O	2.33	0.62
1:A:1299:PHE:HD2	6:A:2406:Y01:HAA3	1.65	0.62
1:A:1491:ASN:ND2	1:A:1582:ARG:HD3	2.14	0.62
3:D:436:LEU:HD21	3:D:482:GLN:HG2	1.81	0.62
3:D:859:LEU:HD21	3:D:867:TYR:HB3	1.81	0.62
1:A:91:PHE:CG	1:A:91:PHE:O	2.53	0.61
1:A:1617:LEU:HD22	1:A:1713:LEU:HD12	1.81	0.61
1:A:1299:PHE:CD2	6:A:2406:Y01:HAA3	2.36	0.61
1:A:1357:ASN:OD1	6:A:2408:Y01:HBF	2.01	0.61
1:A:1769:THR:O	1:A:1779:LYS:HA	2.01	0.61
3:D:824:ASN:HD21	5:F:1:NAG:H61	1.64	0.61
1:A:1176:VAL:HG11	1:A:1647:ARG:NH1	2.16	0.61
1:A:383:TYR:CE1	2:B:392:ASN:HA	2.36	0.60
1:A:386:TRP:HE1	2:B:394:LEU:HA	1.66	0.60
1:A:1760:HIS:ND1	1:A:1802:THR:HG22	2.16	0.60
3:D:976:THR:HB	3:D:1035:GLU:HG3	1.83	0.60
3:D:246:GLN:HE22	3:D:445:GLN:HB3	1.65	0.60
3:D:421:ILE:O	3:D:425:GLU:HG2	2.02	0.60
1:A:689:PHE:N	1:A:689:PHE:CD1	2.69	0.60
3:D:363:ASP:OD1	3:D:364:GLY:N	2.34	0.60
1:A:180:PHE:HB3	1:A:183:HIS:CD2	2.36	0.60
3:D:660:PHE:HD1	3:D:741:THR:HG23	1.67	0.60
2:B:353:GLN:HB3	2:B:357:LYS:HZ1	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2412:Y01:HAB2	6:A:2413:Y01:HAB3	1.84	0.59
1:A:547:VAL:HG11	1:A:572:ARG:HG3	1.84	0.59
2:B:345:LYS:N	2:B:389:LEU:O	2.35	0.59
3:D:37:VAL:HG13	3:D:1008:LEU:HD22	1.83	0.59
3:D:413:ILE:HG12	3:D:422:ASN:HD22	1.67	0.59
3:D:710:GLY:HA2	3:D:713:ASN:HD21	1.67	0.59
1:A:1523:LEU:O	1:A:1527:LEU:HB2	2.02	0.58
1:A:89:PRO:CB	1:A:90:PRO:HD3	2.19	0.58
3:D:459:VAL:HG12	3:D:493:SER:HA	1.84	0.58
3:D:640:THR:HA	3:D:643:ARG:HG2	1.85	0.58
1:A:1471:VAL:HG23	1:A:1472:TRP:N	2.17	0.58
1:A:357:GLU:HG3	1:A:360:ARG:HH12	1.68	0.58
1:A:693:THR:HG22	1:A:693:THR:O	2.02	0.58
1:A:1357:ASN:HB3	1:A:1360:TRP:HD1	1.68	0.58
3:D:147:PRO:HB3	3:D:163:HIS:CE1	2.38	0.58
3:D:744:TYR:O	3:D:746:LYS:HD3	2.04	0.58
3:D:676:ASN:ND2	3:D:756:PRO:HB3	2.19	0.57
1:A:1658:ARG:NH1	1:A:1668:ILE:HD11	2.19	0.57
1:A:466:ARG:O	1:A:470:ARG:NH1	2.37	0.57
1:A:673:VAL:HA	1:A:677:MET:HE3	1.86	0.57
3:D:108:GLN:NE2	4:C:1:NAG:HN2	2.01	0.57
1:A:1461:PRO:HD3	1:A:1472:TRP:CD2	2.40	0.57
1:A:1868:ILE:HG13	1:A:1869:TYR:H	1.70	0.57
1:A:190:ARG:HB3	1:A:193:ARG:NH1	2.20	0.57
3:D:123:VAL:HG12	3:D:143:GLN:HB3	1.87	0.57
1:A:685:VAL:HG12	1:A:685:VAL:O	2.03	0.57
1:A:380:LEU:HD12	2:B:351:VAL:HG23	1.87	0.56
1:A:534:LEU:HA	1:A:537:HIS:CE1	2.40	0.56
3:D:204:LEU:HD11	3:D:493:SER:HB2	1.87	0.56
2:B:346:ILE:HD12	2:B:352:LEU:HD12	1.88	0.56
1:A:368:MET:SD	1:A:371:ARG:NH1	2.77	0.56
1:A:386:TRP:HE3	2:B:248:MET:SD	2.27	0.56
1:A:463:ARG:NH1	1:A:470:ARG:HH12	2.04	0.56
1:A:704:ASP:OD2	10:A:2416:TOR:HAM	2.05	0.56
1:A:1472:TRP:HB2	1:A:1531:ALA:O	2.05	0.56
1:A:1763:GLU:O	1:A:1767:MET:N	2.38	0.56
3:D:334:LYS:HZ3	3:D:369:ALA:HA	1.70	0.56
3:D:651:ASP:OD1	3:D:652:ASN:N	2.39	0.56
1:A:1188:TYR:HA	1:A:1191:TYR:HD2	1.69	0.56
1:A:1360:TRP:O	1:A:1364:THR:HG23	2.05	0.56
1:A:1353:PHE:CE2	1:A:1670:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:TYR:CD1	6:A:2401:Y01:HBD	2.40	0.56
1:A:383:TYR:HE2	2:B:346:ILE:HG12	1.71	0.56
1:A:1354:HIS:O	1:A:1364:THR:HG21	2.06	0.56
3:D:848:MET:N	3:D:1019:GLU:OE1	2.39	0.56
3:D:237:ASP:OD2	3:D:420:ARG:NH2	2.37	0.56
1:A:258:ILE:O	1:A:258:ILE:HG13	2.06	0.55
3:D:352:ALA:O	3:D:354:CYS:N	2.39	0.55
3:D:285:ASP:O	3:D:309:GLN:NE2	2.35	0.55
3:D:820:SER:O	3:D:823:GLU:HG3	2.06	0.55
1:A:1180:SER:OG	1:A:1181:GLU:N	2.37	0.55
6:A:2412:Y01:HAP1	6:A:2417:Y01:HAC2	1.89	0.55
1:A:383:TYR:CE2	2:B:346:ILE:HG12	2.41	0.55
1:A:1182:ARG:O	1:A:1186:LEU:HG	2.07	0.55
1:A:223:GLN:NE2	1:A:226:LEU:HD12	2.20	0.55
3:D:317:VAL:HG21	3:D:1043:PRO:HG2	1.87	0.55
3:D:646:GLU:HA	3:D:649:LYS:NZ	2.21	0.55
1:A:1384:VAL:HG13	1:A:1396:ARG:HD2	1.87	0.55
3:D:599:TYR:O	3:D:980:GLN:NE2	2.40	0.55
1:A:379:GLU:OE2	2:B:348:SER:OG	2.24	0.55
2:B:357:LYS:HD2	2:B:367:LEU:HD22	1.89	0.55
1:A:1521:PHE:O	1:A:1524:GLU:HB2	2.07	0.55
3:D:780:PHE:CE2	3:D:873:ARG:HD2	2.42	0.55
1:A:695:LEU:O	1:A:695:LEU:HG	2.08	0.54
1:A:1473:HIS:O	1:A:1475:VAL:N	2.39	0.54
1:A:1487:MET:HG3	1:A:1520:VAL:HG11	1.89	0.54
1:A:1360:TRP:CZ2	7:A:2409:R16:H282	2.42	0.54
1:A:1502:ALA:HB3	1:A:1507:GLU:HG2	1.89	0.54
1:A:151:HIS:HB3	1:A:154:SER:HB3	1.89	0.54
1:A:1459:TYR:HD1	1:A:1472:TRP:HE1	1.55	0.54
1:A:1303:PHE:HE1	6:A:2406:Y01:HAA2	1.71	0.54
1:A:1449:PHE:CE2	1:A:1741:LEU:HD23	2.43	0.54
1:A:331:PHE:O	1:A:335:ILE:HG12	2.06	0.54
1:A:1757:GLY:O	1:A:1759:ILE:HG22	2.08	0.54
1:A:1528:LYS:O	1:A:1532:PHE:N	2.40	0.54
1:A:1654:MET:HG2	6:A:2410:Y01:HAV2	1.89	0.54
3:D:970:SER:OG	3:D:971:LYS:N	2.41	0.54
1:A:205:PRO:HA	1:A:208:GLN:HG3	1.89	0.53
3:D:886:LEU:HD23	3:D:889:ILE:HD12	1.90	0.53
1:A:1259:VAL:O	1:A:1262:VAL:HG12	2.08	0.53
1:A:190:ARG:HB3	1:A:193:ARG:HH12	1.73	0.53
1:A:1410:PHE:HB2	1:A:1411:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:VAL:HG21	2:B:327:ASN:HA	1.91	0.53
3:D:68:TYR:CE1	3:D:631:ILE:HD12	2.43	0.53
1:A:685:VAL:O	1:A:685:VAL:CG1	2.56	0.53
1:A:1741:LEU:HD11	1:A:1809:LEU:HD11	1.90	0.53
2:B:356:ILE:HD12	2:B:370:GLN:OE1	2.08	0.53
1:A:777:VAL:HG22	1:A:1428:GLU:HG2	1.89	0.53
1:A:1535:LEU:HD11	1:A:1539:ARG:HH21	1.72	0.53
1:A:1788:LYS:HA	1:A:1791:VAL:HG12	1.91	0.53
3:D:660:PHE:CD1	3:D:741:THR:HG23	2.42	0.53
1:A:357:GLU:HG3	1:A:360:ARG:NH1	2.24	0.53
1:A:568:ILE:HG13	1:A:568:ILE:O	2.09	0.53
2:B:243:GLU:HG3	2:B:359:ARG:HG2	1.91	0.53
3:D:182:GLU:HG3	3:D:212:THR:HG21	1.90	0.53
3:D:509:ASN:HB2	3:D:624:PRO:HG2	1.90	0.53
3:D:537:PRO:HB3	3:D:972:GLN:OE1	2.10	0.52
3:D:593:LYS:HG3	3:D:980:GLN:HE22	1.74	0.52
1:A:1481:GLU:O	1:A:1484:ILE:HG22	2.10	0.52
2:B:350:LYS:NZ	2:B:354:ARG:HH21	2.07	0.52
1:A:540:PHE:HB2	1:A:578:ARG:NH2	2.21	0.52
3:D:57:LEU:HB2	3:D:715:LEU:HD22	1.92	0.52
3:D:735:VAL:HG23	3:D:741:THR:HB	1.92	0.52
3:D:850:CYS:H	3:D:863:ASN:ND2	2.07	0.52
1:A:325:THR:HG23	1:A:326:TRP:CD1	2.44	0.52
1:A:689:PHE:N	1:A:689:PHE:HD1	2.07	0.52
3:D:243:TRP:HB3	3:D:461:THR:HG21	1.92	0.52
1:A:1794:ASN:HB3	1:A:1864:THR:HG21	1.91	0.52
3:D:560:ASP:OD1	3:D:561:PHE:N	2.42	0.52
1:A:1803:VAL:HG11	1:A:1865:VAL:HG21	1.92	0.52
3:D:582:GLU:O	3:D:609:TRP:NE1	2.43	0.52
3:D:423:THR:O	3:D:426:TYR:CD2	2.63	0.52
6:A:2412:Y01:HAK1	6:A:2417:Y01:CAS	2.39	0.52
1:A:647:ILE:HG21	7:A:2407:R16:H382	1.92	0.51
1:A:1744:PHE:CD2	1:A:1809:LEU:HD13	2.45	0.51
1:A:364:ARG:O	1:A:368:MET:HG2	2.10	0.51
1:A:1471:VAL:O	1:A:1473:HIS:N	2.44	0.51
3:D:561:PHE:HE1	3:D:565:GLU:OE2	1.93	0.51
1:A:772:ARG:HD3	1:A:773:HIS:N	2.25	0.51
1:A:1666:GLN:HG3	1:A:1667:GLU:N	2.24	0.51
3:D:775:PHE:CD1	3:D:794:VAL:HG22	2.45	0.51
3:D:788:TYR:HA	3:D:818:VAL:HG11	1.92	0.51
3:D:168:ILE:HG12	3:D:214:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:260:VAL:O	3:D:295:ASN:HB3	2.10	0.51
1:A:332:ILE:HB	1:A:333:PRO:HD3	1.93	0.51
3:D:511:TYR:OH	3:D:565:GLU:OE1	2.28	0.51
3:D:644:TYR:O	3:D:647:THR:OG1	2.26	0.51
1:A:240:LEU:O	1:A:244:SER:HB2	2.11	0.50
3:D:250:SER:HB3	3:D:1059:CYS:HB2	1.94	0.50
3:D:573:GLU:OE1	3:D:586:LYS:NZ	2.44	0.50
1:A:1179:ASN:OD1	1:A:1184:LYS:HD2	2.11	0.50
2:B:306:ILE:HA	2:B:309:ILE:HD12	1.94	0.50
3:D:854:ASP:HB3	3:D:1013:LEU:HD23	1.93	0.50
3:D:224:VAL:HG13	3:D:225:ASP:H	1.77	0.50
1:A:168:VAL:O	1:A:172:ILE:HG12	2.11	0.50
1:A:1402:PHE:HA	6:A:2406:Y01:HAK2	1.94	0.50
3:D:240:ARG:HG3	3:D:424:GLN:OE1	2.11	0.50
1:A:1787:TYR:HE1	1:A:1870:ALA:HA	1.77	0.50
1:A:1790:LEU:HA	1:A:1793:MET:HG3	1.93	0.50
1:A:490:THR:HG21	1:A:573:ALA:HB2	1.94	0.50
3:D:99:ARG:HD2	3:D:195:LYS:NZ	2.27	0.50
1:A:466:ARG:NH1	1:A:528:TYR:O	2.44	0.50
6:A:2411:Y01:HAE2	6:A:2411:Y01:HAO1	1.93	0.50
11:D:1203:NAG:O7	11:D:1203:NAG:O3	2.26	0.50
3:D:357:ILE:HD11	3:D:430:LEU:HD11	1.94	0.50
3:D:712:THR:HG22	3:D:742:ARG:HD2	1.94	0.50
1:A:1506:TYR:HA	6:A:2401:Y01:HAK1	1.93	0.49
1:A:309:GLU:HG3	1:A:659:TRP:CD1	2.47	0.49
3:D:470:THR:HG21	4:C:1:NAG:H5	1.95	0.49
1:A:1402:PHE:HB2	6:A:2406:Y01:CAK	2.42	0.49
3:D:41:GLN:NE2	3:D:42:GLU:OE2	2.45	0.49
3:D:852:ILE:HD13	3:D:1015:PHE:HA	1.93	0.49
1:A:106:LEU:HD23	1:A:619:LEU:HD13	1.95	0.49
1:A:145:ALA:O	1:A:146:LEU:HD12	2.13	0.49
1:A:495:ILE:HG22	6:A:2408:Y01:HAE2	1.94	0.49
1:A:1373:GLY:HA3	1:A:1666:GLN:HE22	1.76	0.49
1:A:1465:HIS:CG	1:A:1466:THR:N	2.79	0.49
3:D:885:HIS:CD2	3:D:994:LEU:HA	2.47	0.49
1:A:224:ILE:O	1:A:228:LEU:N	2.36	0.49
3:D:849:ASP:OD1	3:D:864:HIS:HB2	2.11	0.49
1:A:86:ILE:HB	1:A:141:ILE:HD11	1.94	0.49
1:A:176:ALA:HA	1:A:179:HIS:CE1	2.48	0.49
1:A:1497:MET:HB3	1:A:1506:TYR:OH	2.13	0.49
1:A:1796:PRO:HD3	1:A:1858:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2406:Y01:HAV1	6:A:2406:Y01:OAG	2.13	0.49
3:D:407:LYS:HE2	3:D:1068:TYR:CZ	2.48	0.49
1:A:186:LEU:HD12	1:A:187:ARG:N	2.27	0.49
1:A:1385:THR:HG22	1:A:1395:ASN:HD22	1.77	0.49
1:A:1846:LEU:HB2	1:A:1851:LEU:HD13	1.95	0.49
3:D:421:ILE:O	3:D:424:GLN:HG2	2.13	0.49
3:D:791:GLY:HA3	3:D:816:ILE:O	2.13	0.49
3:D:893:ALA:HB2	3:D:984:ASP:OD1	2.12	0.49
1:A:470:ARG:HA	1:A:473:VAL:HG12	1.94	0.49
3:D:710:GLY:HA2	3:D:713:ASN:ND2	2.28	0.49
1:A:1335:ASP:O	1:A:1341:MET:HA	2.13	0.49
3:D:721:SER:HA	3:D:744:TYR:OH	2.13	0.49
1:A:88:TRP:CB	1:A:89:PRO:HD2	2.43	0.48
1:A:263:ASP:HB3	1:A:264:PRO:HD3	1.94	0.48
1:A:673:VAL:HG13	1:A:673:VAL:O	2.13	0.48
3:D:997:GLY:N	3:D:1026:CYS:SG	2.78	0.48
1:A:691:ASN:OD1	1:A:691:ASN:O	2.31	0.48
1:A:1591:TYR:HB2	1:A:1594:ARG:HH21	1.78	0.48
1:A:469:ILE:HG21	1:A:529:GLY:HA3	1.94	0.48
1:A:1673:LEU:O	1:A:1695:GLY:HA3	2.13	0.48
1:A:1761:TYR:O	1:A:1764:MET:HB2	2.13	0.48
3:D:166:VAL:HG11	3:D:183:LEU:HD21	1.95	0.48
1:A:1467:PHE:CA	1:A:1470:ARG:HB3	2.37	0.48
1:A:1499:TYR:CZ	1:A:1502:ALA:HA	2.48	0.48
3:D:994:LEU:HD22	3:D:1001:ARG:HG3	1.96	0.48
1:A:1454:LYS:NZ	1:A:1756:CYS:SG	2.77	0.48
3:D:56:GLN:O	3:D:60:ILE:HG13	2.13	0.48
3:D:298:ALA:HB2	3:D:336:GLY:HA2	1.95	0.48
3:D:656:SER:HA	3:D:716:VAL:HG11	1.95	0.48
1:A:91:PHE:O	1:A:91:PHE:CD2	2.67	0.48
2:B:329:PRO:HB2	2:B:384:MET:HB3	1.96	0.48
1:A:386:TRP:HE1	2:B:394:LEU:CA	2.26	0.48
3:D:791:GLY:CA	3:D:816:ILE:O	2.62	0.48
3:D:852:ILE:O	3:D:853:LEU:HD23	2.13	0.48
1:A:88:TRP:CE2	1:A:90:PRO:CD	2.95	0.47
1:A:1658:ARG:HH11	1:A:1668:ILE:HD11	1.79	0.47
1:A:232:ILE:HG12	1:A:306:ILE:HD12	1.97	0.47
1:A:681:ILE:HG22	1:A:681:ILE:O	2.13	0.47
3:D:736:THR:HG22	3:D:740:ILE:O	2.13	0.47
3:D:824:ASN:ND2	5:F:1:NAG:H61	2.29	0.47
3:D:224:VAL:HG13	3:D:225:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:ILE:HA	3:D:419:ILE:HG12	1.96	0.47
3:D:873:ARG:CZ	3:D:877:GLU:HG3	2.45	0.47
1:A:1646:PHE:CZ	1:A:1655:LEU:HD22	2.49	0.47
6:A:2410:Y01:HAN1	6:A:2410:Y01:HAC3	1.95	0.47
3:D:753:GLN:OE1	3:D:753:GLN:N	2.47	0.47
1:A:1358:ILE:HG13	1:A:1358:ILE:O	2.14	0.47
3:D:413:ILE:HG21	3:D:419:ILE:HD13	1.95	0.47
3:D:469:ILE:HG22	3:D:469:ILE:O	2.15	0.47
3:D:870:GLN:NE2	3:D:878:ILE:HG12	2.29	0.47
1:A:155:TYR:CD2	1:A:156:LEU:HD22	2.47	0.47
1:A:701:ILE:O	1:A:705:ASN:ND2	2.47	0.47
1:A:705:ASN:ND2	10:A:2416:TOR:OAS	2.46	0.47
1:A:1464:ARG:HA	1:A:1464:ARG:NE	2.29	0.47
1:A:1748:TRP:HA	1:A:1767:MET:CE	2.44	0.47
2:B:252:LEU:HD21	2:B:401:LEU:HD22	1.97	0.47
2:B:332:LEU:HD23	2:B:332:LEU:O	2.15	0.47
3:D:254:MET:HE3	3:D:283:LEU:HD21	1.97	0.47
3:D:988:LYS:NZ	3:D:1009:MET:SD	2.87	0.47
1:A:1742:ASP:OD1	1:A:1742:ASP:N	2.46	0.47
1:A:214:ILE:HG13	1:A:606:LEU:HD11	1.97	0.47
1:A:1314:LYS:HB3	1:A:1384:VAL:CG2	2.44	0.47
1:A:1727:GLU:OE1	1:A:1727:GLU:HA	2.15	0.47
6:A:2414:Y01:HAO1	6:A:2414:Y01:HAP1	1.37	0.47
2:B:255:PHE:HA	2:B:258:HIS:ND1	2.29	0.47
3:D:285:ASP:OD2	3:D:558:THR:HG21	2.14	0.47
3:D:604:ASN:OD1	11:D:1205:NAG:N2	2.48	0.47
1:A:593:VAL:HG21	7:A:2419:R16:H301	1.97	0.47
1:A:1703:PHE:O	1:A:1707:ILE:HG12	2.15	0.47
3:D:556:PRO:HB2	3:D:558:THR:HG23	1.97	0.47
1:A:1431:ASP:OD1	1:A:1431:ASP:N	2.48	0.46
2:B:327:ASN:O	2:B:377:LEU:HD21	2.15	0.46
2:B:342:VAL:HG13	2:B:387:ILE:HB	1.97	0.46
2:B:350:LYS:HZ3	2:B:354:ARG:HH21	1.61	0.46
3:D:149:PHE:HB3	3:D:158:GLN:HB3	1.97	0.46
3:D:218:TYR:HB3	3:D:219:PRO:HD3	1.97	0.46
3:D:683:PHE:CE2	3:D:687:ILE:HD11	2.50	0.46
3:D:799:GLU:OE1	3:D:808:LYS:HE2	2.15	0.46
1:A:1247:LYS:CB	1:A:1250:ASP:OD2	2.58	0.46
1:A:1472:TRP:CD2	1:A:1472:TRP:O	2.69	0.46
1:A:1743:GLU:O	1:A:1747:VAL:HG22	2.16	0.46
1:A:1768:LEU:HB3	1:A:1777:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:MET:O	1:A:1778:GLY:HA2	2.15	0.46
3:D:896:LYS:HB3	3:D:977:GLU:OE2	2.15	0.46
1:A:1412:PHE:O	1:A:1416:ASN:ND2	2.39	0.46
1:A:1473:HIS:O	1:A:1476:VAL:N	2.48	0.46
3:D:723:GLN:NE2	3:D:725:ASN:O	2.44	0.46
1:A:219:VAL:N	1:A:220:PRO:HD2	2.31	0.46
1:A:1164:ALA:O	1:A:1168:ILE:HG12	2.16	0.46
1:A:1243:LEU:HD21	1:A:1246:ASN:OD1	2.15	0.46
1:A:1324:ASP:O	1:A:1325:THR:OG1	2.30	0.46
1:A:1499:TYR:CD2	6:A:2413:Y01:HAR2	2.51	0.46
1:A:1795:MET:HA	1:A:1858:PRO:HG3	1.97	0.46
1:A:1796:PRO:CD	1:A:1856:PRO:HB2	2.45	0.46
2:B:244:VAL:O	2:B:248:MET:HG2	2.16	0.46
3:D:521:VAL:HG22	3:D:559:LEU:O	2.15	0.46
1:A:654:LEU:C	1:A:656:GLY:N	2.69	0.46
2:B:350:LYS:O	2:B:354:ARG:HG3	2.15	0.46
1:A:690:GLY:O	1:A:694:LEU:HB2	2.15	0.46
1:A:1229:VAL:CG1	1:A:1267:LYS:HZ1	2.27	0.46
1:A:1476:VAL:HG12	1:A:1477:SER:N	2.30	0.46
3:D:179:VAL:HG13	3:D:214:LEU:HD21	1.98	0.46
3:D:646:GLU:HA	3:D:649:LYS:HZ2	1.81	0.46
1:A:524:SER:O	1:A:528:TYR:N	2.46	0.46
1:A:1474:PHE:CE1	1:A:1480:PHE:HB2	2.50	0.46
2:B:353:GLN:HB3	2:B:357:LYS:HZ3	1.77	0.46
3:D:870:GLN:O	3:D:870:GLN:HG3	2.16	0.46
1:A:91:PHE:CZ	1:A:138:GLU:OE1	2.68	0.46
1:A:693:THR:O	1:A:693:THR:CG2	2.64	0.46
1:A:772:ARG:HD3	1:A:773:HIS:H	1.80	0.46
1:A:1151:ASN:O	1:A:1152:LEU:HD23	2.15	0.46
1:A:1642:ARG:H	1:A:1642:ARG:HG2	1.49	0.46
3:D:654:GLU:HA	3:D:746:LYS:HE3	1.97	0.46
1:A:1304:ALA:HB3	1:A:1358:ILE:HD11	1.97	0.46
3:D:469:ILE:HG23	3:D:472:GLN:HG3	1.98	0.46
3:D:788:TYR:OH	3:D:869:ASN:HA	2.16	0.46
3:D:850:CYS:H	3:D:863:ASN:CG	2.18	0.46
1:A:1471:VAL:O	1:A:1472:TRP:C	2.53	0.45
1:A:1551:ILE:O	1:A:1555:THR:HG22	2.15	0.45
6:A:2401:Y01:HAM2	6:A:2401:Y01:HBC	1.49	0.45
2:B:234:LEU:HD13	2:B:253:PHE:CE1	2.50	0.45
1:A:526:LYS:HB3	1:A:535:TYR:HE1	1.81	0.45
3:D:123:VAL:HA	3:D:143:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:882:LEU:O	3:D:886:LEU:HG	2.17	0.45
1:A:1316:PHE:CE1	1:A:1350:ARG:HG3	2.51	0.45
3:D:149:PHE:HD1	3:D:160:SER:HB3	1.81	0.45
3:D:379:ASP:OD1	3:D:379:ASP:N	2.40	0.45
3:D:978:GLN:NE2	3:D:1035:GLU:OE2	2.49	0.45
1:A:1504:CYS:SG	1:A:1505:THR:N	2.87	0.45
3:D:640:THR:O	3:D:643:ARG:HG2	2.16	0.45
3:D:1064:VAL:HG13	3:D:1065:LEU:HD22	1.98	0.45
3:D:40:MET:O	3:D:44:LEU:HD23	2.16	0.45
3:D:56:GLN:OE1	3:D:56:GLN:N	2.47	0.45
1:A:300:LEU:HD13	1:A:684:ILE:HD11	1.99	0.45
3:D:193:PHE:CD2	3:D:218:TYR:HB2	2.52	0.45
1:A:474:LYS:HB3	1:A:474:LYS:HE2	1.68	0.45
1:A:1488:ILE:HD13	1:A:1585:LYS:HB3	1.99	0.45
1:A:1621:TYR:O	1:A:1702:TYR:OH	2.26	0.45
2:B:308:ARG:HA	2:B:311:GLU:HG3	1.98	0.45
1:A:1465:HIS:CG	1:A:1466:THR:H	2.35	0.45
1:A:1840:LEU:HD12	1:A:1844:PRO:HA	1.99	0.45
2:B:234:LEU:HG	2:B:342:VAL:HB	1.99	0.45
3:D:54:VAL:O	3:D:58:VAL:HG23	2.16	0.45
3:D:462:GLY:O	3:D:489:GLY:HA2	2.17	0.45
3:D:768:LEU:HD23	3:D:768:LEU:HA	1.82	0.45
3:D:892:TYR:HE1	3:D:983:PHE:CE1	2.35	0.45
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.81	0.45
1:A:485:LEU:HD21	1:A:518:LEU:HD22	1.99	0.45
1:A:1785:VAL:HA	1:A:1788:LYS:HE3	1.99	0.45
1:A:1857:MET:HE3	1:A:1859:LYS:HG3	1.98	0.44
3:D:482:GLN:HE22	3:D:1067:ASP:N	2.15	0.44
3:D:526:ASN:ND2	3:D:564:ALA:O	2.43	0.44
3:D:886:LEU:HA	3:D:889:ILE:HD12	1.99	0.44
1:A:1243:LEU:HB3	1:A:1247:LYS:NZ	2.33	0.44
1:A:1748:TRP:HA	1:A:1767:MET:HE3	1.99	0.44
3:D:506:LEU:O	3:D:759:TYR:OH	2.22	0.44
1:A:1505:THR:HG23	6:A:2401:Y01:HAV2	1.98	0.44
6:A:2413:Y01:HBB	6:A:2413:Y01:HAE2	1.83	0.44
3:D:152:ASP:OD1	3:D:153:ALA:N	2.50	0.44
3:D:169:PRO:HG2	3:D:172:ILE:HD12	1.98	0.44
3:D:425:GLU:O	3:D:428:ASP:HB3	2.17	0.44
3:D:29:SER:HB3	3:D:32:THR:CG2	2.47	0.44
3:D:33:ILE:HG22	3:D:36:TRP:CE3	2.53	0.44
3:D:1031:LEU:HD23	3:D:1031:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:653:PHE:CE1	3:D:659:THR:HG22	2.53	0.44
1:A:651:PHE:O	1:A:655:THR:HG23	2.17	0.44
1:A:1461:PRO:HD3	1:A:1472:TRP:CE2	2.53	0.44
2:B:308:ARG:O	2:B:311:GLU:HG3	2.17	0.44
3:D:615:THR:HG22	3:D:616:ASP:N	2.33	0.44
1:A:208:GLN:O	1:A:212:LYS:HG2	2.18	0.44
1:A:1168:ILE:HG21	6:A:2411:Y01:HAN1	2.00	0.44
6:A:2410:Y01:OAG	6:A:2410:Y01:HAR1	2.18	0.44
3:D:474:GLU:O	3:D:476:LYS:HG3	2.17	0.44
1:A:254:ASN:OD1	1:A:278:GLU:HB2	2.17	0.44
1:A:1440:GLU:HG2	1:A:1838:GLU:HG2	1.99	0.44
1:A:1528:LYS:HA	1:A:1531:ALA:HB3	2.00	0.44
1:A:136:CYS:HB3	1:A:172:ILE:HD11	2.00	0.44
1:A:383:TYR:HE1	2:B:392:ASN:HA	1.81	0.44
1:A:565:SER:O	1:A:567:GLY:N	2.51	0.44
1:A:610:LEU:HD13	1:A:694:LEU:HD21	2.00	0.44
1:A:1828:ARG:NH2	1:A:1858:PRO:O	2.51	0.44
3:D:75:ALA:HB2	3:D:623:LEU:HD12	1.98	0.44
3:D:193:PHE:CG	3:D:218:TYR:HB2	2.53	0.44
1:A:95:ILE:O	1:A:98:THR:HG22	2.18	0.43
1:A:1374:TRP:CD1	1:A:1375:PRO:HD3	2.53	0.43
1:A:1613:LEU:HD12	1:A:1613:LEU:HA	1.75	0.43
3:D:360:LEU:HD23	3:D:386:THR:HG22	2.00	0.43
3:D:369:ALA:HB1	3:D:372:ILE:HG22	1.98	0.43
1:A:484:SER:O	1:A:488:LEU:HD23	2.18	0.43
1:A:1163:ILE:HD13	1:A:1197:PHE:CZ	2.53	0.43
1:A:1459:TYR:CD1	1:A:1459:TYR:C	2.91	0.43
1:A:1655:LEU:HD21	1:A:1668:ILE:HG21	2.00	0.43
3:D:178:ILE:HD12	3:D:178:ILE:H	1.83	0.43
1:A:1229:VAL:HG11	1:A:1267:LYS:NZ	2.29	0.43
1:A:1772:SER:C	1:A:1774:PRO:HD2	2.38	0.43
1:A:1796:PRO:HD2	1:A:1856:PRO:HB2	1.99	0.43
3:D:261:SER:O	3:D:327:ALA:HB1	2.17	0.43
3:D:854:ASP:OD1	3:D:854:ASP:N	2.51	0.43
1:A:1385:THR:O	1:A:1386:GLU:HG3	2.18	0.43
1:A:1683:THR:HG22	1:A:1683:THR:O	2.17	0.43
1:A:1789:ARG:NH1	1:A:1815:THR:O	2.44	0.43
1:A:1848:GLN:HA	1:A:1851:LEU:HB3	2.00	0.43
3:D:254:MET:CE	3:D:283:LEU:HD21	2.48	0.43
3:D:260:VAL:O	3:D:260:VAL:HG23	2.18	0.43
1:A:160:TRP:O	1:A:163:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:LEU:HD23	1:A:609:LEU:HA	1.82	0.43
2:B:268:ARG:HA	2:B:322:ASP:HB3	2.00	0.43
1:A:314:VAL:O	1:A:318:THR:HG23	2.19	0.43
1:A:1312:LYS:HB3	1:A:1312:LYS:HE2	1.61	0.43
1:A:1449:PHE:HE2	1:A:1738:PRO:HB3	1.84	0.43
6:A:2413:Y01:HAA2	6:A:2413:Y01:HAJ2	1.87	0.43
3:D:366:GLU:HA	3:D:398:PRO:HG2	2.01	0.43
3:D:517:PRO:CG	3:D:616:ASP:HB2	2.46	0.43
3:D:770:ASN:HB3	3:D:772:ASN:OD1	2.18	0.43
3:D:798:VAL:HG12	3:D:800:ILE:HG23	2.01	0.43
1:A:180:PHE:HB3	1:A:183:HIS:NE2	2.34	0.43
1:A:1166:SER:HB2	1:A:1264:ARG:NE	2.32	0.43
1:A:1597:LEU:HD23	1:A:1597:LEU:HA	1.69	0.43
3:D:407:LYS:HE2	3:D:1068:TYR:CE2	2.53	0.43
3:D:432:ARG:HB2	3:D:433:PRO:HD3	2.01	0.43
3:D:554:GLN:OE1	3:D:554:GLN:N	2.51	0.43
3:D:561:PHE:CE1	3:D:565:GLU:OE2	2.70	0.43
1:A:1781:CYS:SG	1:A:1785:VAL:HB	2.59	0.43
2:B:243:GLU:HA	2:B:246:ASP:HB2	2.01	0.43
3:D:52:SER:OG	3:D:54:VAL:HG23	2.18	0.43
3:D:193:PHE:HB3	3:D:218:TYR:CG	2.54	0.43
3:D:481:ASN:OD1	4:C:1:NAG:O6	2.37	0.43
3:D:655:GLU:HB3	3:D:717:GLN:HE22	1.84	0.43
3:D:850:CYS:HB3	3:D:1015:PHE:CZ	2.54	0.43
1:A:177:GLY:O	1:A:181:ASN:N	2.51	0.43
1:A:1764:MET:O	1:A:1767:MET:HB2	2.18	0.43
1:A:1804:HIS:CD2	1:A:1853:LEU:HD21	2.54	0.43
3:D:133:PRO:HA	3:D:146:LYS:HE3	2.01	0.43
3:D:528:GLN:O	3:D:530:LYS:N	2.52	0.43
3:D:734:VAL:HG23	3:D:812:VAL:HG12	1.99	0.43
2:B:227:PRO:HG3	2:B:310:PHE:CE1	2.54	0.43
2:B:243:GLU:CG	2:B:359:ARG:HG2	2.48	0.43
1:A:1243:LEU:HB3	1:A:1247:LYS:HZ3	1.84	0.42
1:A:1804:HIS:NE2	1:A:1853:LEU:HD21	2.33	0.42
2:B:401:LEU:HD12	2:B:401:LEU:HA	1.87	0.42
3:D:595:GLN:HB2	3:D:765:LYS:CE	2.49	0.42
3:D:801:TYR:CZ	3:D:806:LEU:HB3	2.54	0.42
1:A:1449:PHE:CE2	1:A:1738:PRO:HB3	2.54	0.42
1:A:1486:ALA:O	1:A:1490:LEU:HG	2.19	0.42
1:A:1657:PHE:HB2	6:A:2410:Y01:HAK1	2.00	0.42
3:D:104:ALA:HB2	3:D:189:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:386:THR:HB	3:D:399:ILE:HG23	2.01	0.42
1:A:91:PHE:CD2	1:A:91:PHE:C	2.92	0.42
1:A:116:ASP:HB2	3:D:262:GLY:HA3	2.01	0.42
1:A:116:ASP:OD1	1:A:117:LYS:N	2.52	0.42
1:A:1752:ASP:CG	1:A:1754:ALA:HB2	2.39	0.42
3:D:713:ASN:O	3:D:717:GLN:HG2	2.20	0.42
1:A:1261:ARG:O	1:A:1264:ARG:HG3	2.20	0.42
1:A:1366:PHE:O	1:A:1370:THR:HG23	2.20	0.42
1:A:1640:ILE:HA	1:A:1644:ASN:O	2.19	0.42
3:D:52:SER:HB3	3:D:814:ILE:HD11	2.02	0.42
1:A:265:PRO:O	1:A:267:PRO:HD3	2.20	0.42
1:A:386:TRP:CD1	2:B:394:LEU:HB2	2.55	0.42
1:A:1176:VAL:HG13	1:A:1177:LEU:N	2.34	0.42
1:A:1450:ALA:HB1	1:A:1806:THR:OG1	2.20	0.42
1:A:1864:THR:HG1	1:A:1867:LYS:H	1.63	0.42
3:D:69:THR:HB	3:D:71:GLU:OE2	2.19	0.42
3:D:775:PHE:HE2	3:D:1011:THR:OG1	2.02	0.42
3:D:880:PRO:HG3	3:D:1029:ARG:O	2.19	0.42
1:A:781:ARG:HD2	1:A:781:ARG:HA	1.75	0.42
1:A:1444:ARG:O	1:A:1447:ILE:HG22	2.19	0.42
1:A:262:PHE:HE1	1:A:277:TYR:CZ	2.37	0.42
1:A:688:LEU:HD23	1:A:688:LEU:HA	1.72	0.42
1:A:772:ARG:CZ	1:A:774:HIS:H	2.32	0.42
1:A:1440:GLU:HB2	1:A:1842:ILE:HD11	2.02	0.42
3:D:830:ILE:HD12	3:D:831:ARG:HH21	1.85	0.42
1:A:112:LEU:CD2	1:A:118:THR:HG23	2.49	0.42
1:A:534:LEU:HA	1:A:537:HIS:ND1	2.35	0.42
3:D:892:TYR:HE1	3:D:983:PHE:HE1	1.68	0.42
1:A:263:ASP:O	1:A:265:PRO:HD3	2.20	0.42
1:A:652:GLN:O	1:A:656:GLY:N	2.53	0.42
1:A:772:ARG:NH1	1:A:774:HIS:H	2.17	0.42
1:A:1447:ILE:HG12	1:A:1741:LEU:HD22	2.02	0.42
2:B:376:LYS:HA	2:B:379:GLN:OE1	2.19	0.42
3:D:99:ARG:HD2	3:D:195:LYS:HZ3	1.85	0.42
3:D:577:LYS:HG2	3:D:609:TRP:HZ2	1.84	0.42
1:A:162:VAL:O	1:A:166:ILE:HG12	2.19	0.41
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.77	0.41
1:A:777:VAL:HG23	1:A:1426:PHE:O	2.20	0.41
1:A:1611:CYS:HB2	6:A:2410:Y01:HAN2	2.01	0.41
2:B:381:PRO:HA	2:B:382:PRO:HD3	1.93	0.41
3:D:44:LEU:HD21	3:D:821:TRP:NE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:494:LEU:O	3:D:498:LYS:HG3	2.19	0.41
1:A:84:LYS:HB3	1:A:84:LYS:HE3	1.86	0.41
1:A:386:TRP:NE1	2:B:394:LEU:HA	2.35	0.41
1:A:1343:VAL:O	1:A:1343:VAL:HG13	2.20	0.41
1:A:1472:TRP:HA	1:A:1531:ALA:HB1	2.01	0.41
1:A:1493:VAL:O	1:A:1497:MET:HG3	2.20	0.41
1:A:1691:ASN:C	1:A:1693:ARG:H	2.23	0.41
2:B:329:PRO:HG3	2:B:380:CYS:HB3	2.02	0.41
3:D:509:ASN:OD1	3:D:626:TYR:OH	2.38	0.41
1:A:360:ARG:HE	1:A:362:GLU:CD	2.22	0.41
1:A:1472:TRP:C	1:A:1472:TRP:CE3	2.93	0.41
1:A:1784:LYS:HA	1:A:1787:TYR:HB3	2.02	0.41
2:B:393:GLN:HB3	2:B:395:GLU:OE2	2.20	0.41
1:A:1760:HIS:O	1:A:1761:TYR:HB3	2.20	0.41
1:A:1777:LEU:HD23	1:A:1789:ARG:HD3	2.03	0.41
1:A:1799:GLU:HG3	1:A:1800:ASP:N	2.35	0.41
1:A:1825:GLY:O	1:A:1828:ARG:HG2	2.20	0.41
3:D:148:VAL:HG13	3:D:148:VAL:O	2.20	0.41
3:D:1005:GLY:HA2	3:D:1015:PHE:O	2.20	0.41
1:A:138:GLU:OE1	1:A:138:GLU:HA	2.19	0.41
1:A:232:ILE:HG23	1:A:302:VAL:HG13	2.02	0.41
1:A:1423:ILE:HG23	1:A:1723:MET:CE	2.51	0.41
1:A:1752:ASP:CG	1:A:1763:GLU:HG2	2.41	0.41
1:A:1827:ASP:O	1:A:1830:GLN:NE2	2.53	0.41
2:B:349:PRO:O	2:B:352:LEU:N	2.53	0.41
3:D:197:ARG:HD2	3:D:197:ARG:O	2.20	0.41
3:D:744:TYR:HB3	3:D:745:PRO:HD3	2.02	0.41
3:D:1021:LYS:HA	3:D:1021:LYS:HD2	1.86	0.41
1:A:311:TRP:HE1	1:A:1661:THR:HG21	1.85	0.41
1:A:1354:HIS:CE1	1:A:1360:TRP:CG	3.08	0.41
1:A:1754:ALA:HB1	1:A:1757:GLY:O	2.21	0.41
3:D:363:ASP:HB2	3:D:392:HIS:CD2	2.55	0.41
3:D:501:THR:O	3:D:501:THR:OG1	2.31	0.41
3:D:879:ASP:OD1	3:D:879:ASP:N	2.54	0.41
3:D:880:PRO:HB2	3:D:884:ARG:NH1	2.29	0.41
1:A:1152:LEU:C	1:A:1154:TYR:H	2.23	0.41
1:A:1209:GLY:C	1:A:1210:LEU:HD12	2.41	0.41
2:B:242:TYR:CD1	2:B:370:GLN:NE2	2.89	0.41
3:D:413:ILE:CG2	3:D:419:ILE:HD13	2.50	0.41
3:D:789:GLU:N	3:D:789:GLU:OE1	2.53	0.41
1:A:159:GLY:O	1:A:162:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:ALA:HB3	1:A:1802:THR:OG1	2.20	0.41
3:D:975:ILE:H	3:D:975:ILE:HD12	1.86	0.41
1:A:1179:ASN:HB3	1:A:1683:THR:CG2	2.50	0.41
1:A:1292:ILE:HG13	1:A:1421:LEU:HD11	2.02	0.41
1:A:1467:PHE:O	1:A:1471:VAL:HG22	2.20	0.41
1:A:1820:LYS:HD2	1:A:1835:LEU:HD13	2.02	0.41
6:A:2410:Y01:HAO2	6:A:2410:Y01:HAE2	2.03	0.41
2:B:253:PHE:HD1	2:B:256:LEU:HD12	1.86	0.41
3:D:103:GLU:HG2	3:D:192:VAL:HG21	2.02	0.41
3:D:122:VAL:HG21	3:D:180:LEU:HD22	2.02	0.41
3:D:851:VAL:HG12	3:D:862:ALA:CB	2.51	0.41
3:D:883:MET:HA	3:D:886:LEU:HD12	2.03	0.41
3:D:886:LEU:HB3	3:D:891:VAL:CG1	2.51	0.41
1:A:495:ILE:O	1:A:497:HIS:ND1	2.49	0.41
1:A:538:SER:HB3	1:A:541:ASN:HB2	2.01	0.41
1:A:1772:SER:O	1:A:1774:PRO:HD2	2.21	0.41
3:D:691:THR:N	3:D:692:PRO:HD2	2.36	0.41
1:A:88:TRP:CZ2	1:A:90:PRO:HG2	2.56	0.40
1:A:466:ARG:O	1:A:470:ARG:HD3	2.21	0.40
1:A:1491:ASN:HD21	1:A:1582:ARG:NH1	2.18	0.40
1:A:1606:ALA:O	1:A:1607:LEU:HD23	2.22	0.40
6:A:2406:Y01:HAC2	6:A:2406:Y01:HAJ2	1.77	0.40
3:D:469:ILE:HG23	3:D:469:ILE:HD12	1.78	0.40
2:B:365:LYS:HA	2:B:365:LYS:HD2	1.87	0.40
3:D:164:ALA:HA	3:D:218:TYR:O	2.20	0.40
1:A:360:ARG:NE	1:A:362:GLU:OE1	2.47	0.40
3:D:653:PHE:HE1	3:D:659:THR:H	1.68	0.40
1:A:524:SER:O	1:A:527:MET:N	2.53	0.40
1:A:1537:TYR:HD2	1:A:1538:PHE:CE1	2.40	0.40
6:A:2412:Y01:HAI	6:A:2417:Y01:HAT2	2.02	0.40
3:D:28:PRO:HB2	3:D:33:ILE:HG23	2.03	0.40
3:D:132:ASP:HA	3:D:133:PRO:HD3	1.99	0.40
3:D:515:ILE:HG21	3:D:515:ILE:HD13	1.87	0.40
1:A:333:PRO:O	1:A:337:ILE:HB	2.22	0.40
3:D:883:MET:HA	3:D:886:LEU:HB2	2.02	0.40
3:D:991:SER:HB3	3:D:1004:HIS:ND1	2.37	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	1309/2313 (57%)	1136 (87%)	165 (13%)	8 (1%)	22 57
2	B	158/598 (26%)	144 (91%)	14 (9%)	0	100 100
3	D	947/1103 (86%)	864 (91%)	83 (9%)	0	100 100
All	All	2414/4014 (60%)	2144 (89%)	262 (11%)	8 (0%)	38 70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1504	CYS
1	A	1761	TYR
1	A	1682	THR
1	A	690	GLY
1	A	674	SER
1	A	1474	PHE
1	A	1764	MET
1	A	274	PRO

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	1160/2023 (57%)	1147 (99%)	13 (1%)	70 87
2	B	136/510 (27%)	136 (100%)	0	100 100
3	D	846/971 (87%)	845 (100%)	1 (0%)	92 98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2142/3504 (61%)	2128 (99%)	14 (1%)	80 91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	88	TRP
1	A	89	PRO
1	A	91	PHE
1	A	688	LEU
1	A	689	PHE
1	A	691	ASN
1	A	695	LEU
1	A	696	ASN
1	A	1462	GLN
1	A	1464	ARG
1	A	1467	PHE
1	A	1760	HIS
3	D	1029	ARG

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

Mol	Chain	Res	Type
1	A	102	ASN
1	A	691	ASN
1	A	1291	ASN
1	A	1354	HIS
1	A	1462	GLN
1	A	1491	ASN
1	A	1602	GLN
3	D	108	GLN
3	D	246	GLN
3	D	422	ASN
3	D	676	ASN
3	D	870	GLN
3	D	980	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 monosaccharides 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	$\#\|Z\| > 2$
4	NAG	C	1	4,3	14,14,15	0.84	1 (7%)	17,19,21	0.62	0
4	NAG	C	2	4	14,14,15	0.28	0	17,19,21	0.65	0
4	BMA	C	3	4	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
4	NAG	E	1	4,3	14,14,15	0.71	1 (7%)	17,19,21	0.68	0
4	NAG	E	2	4	14,14,15	0.37	0	17,19,21	0.37	0
4	BMA	E	3	4	11,11,12	0.66	0	15,15,17	1.09	2 (13%)
5	NAG	F	1	5,3	14,14,15	0.83	1 (7%)	17,19,21	1.18	1 (5%)
5	NAG	F	2	5	14,14,15	0.17	0	17,19,21	0.53	0
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.81	1 (6%)

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
4	NAG	C	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	3/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,3	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,3	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-2.99	1.38	1.43
5	F	1	NAG	O5-C1	2.95	1.48	1.43
4	E	1	NAG	O5-C1	-2.27	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C1-O5-C5	4.61	118.44	112.19
4	E	3	BMA	C1-O5-C5	2.35	115.37	112.19
5	F	3	BMA	O2-C2-C3	-2.23	105.67	110.14
4	C	3	BMA	O2-C2-C3	-2.09	105.96	110.14
4	E	3	BMA	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
5	F	1	NAG	C1-C2-N2-C7
4	C	2	NAG	C3-C2-N2-C7
4	C	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6

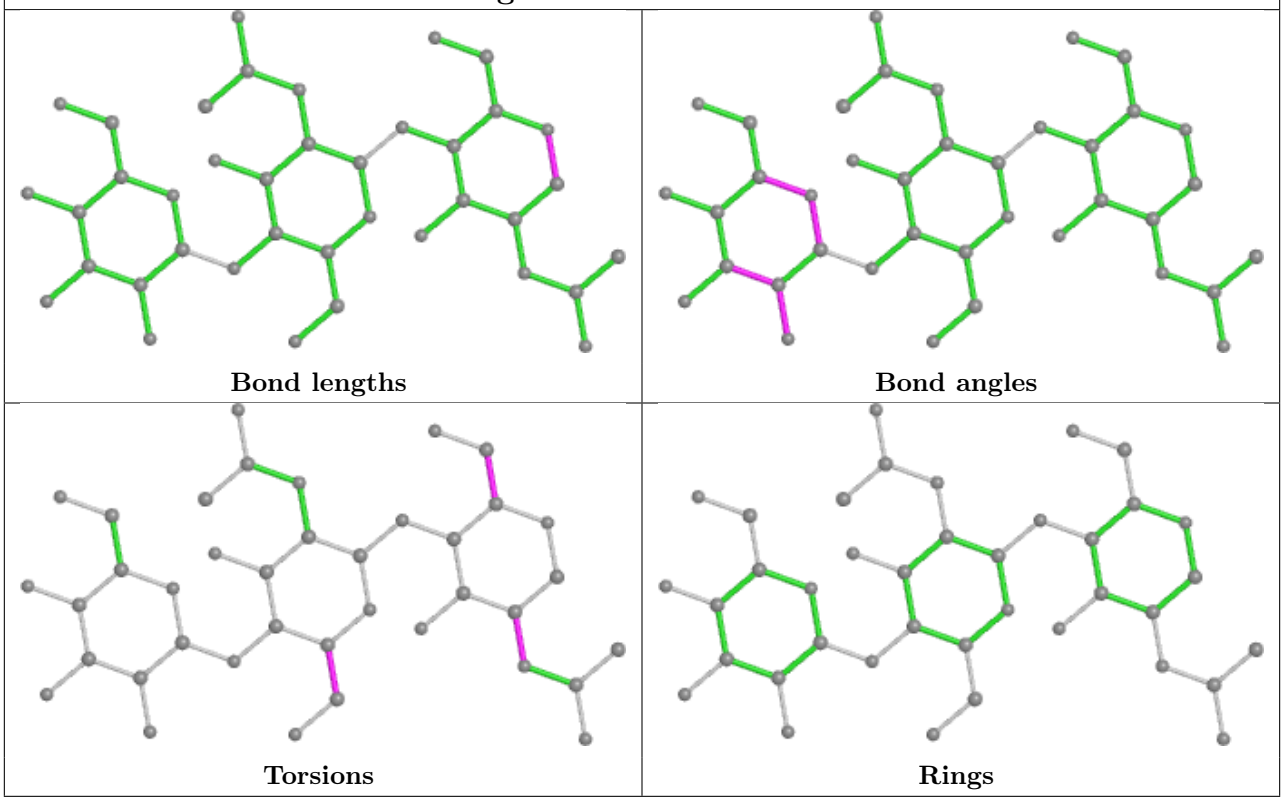
There are no ring outliers.

2 monomers are involved in 6 short contacts:

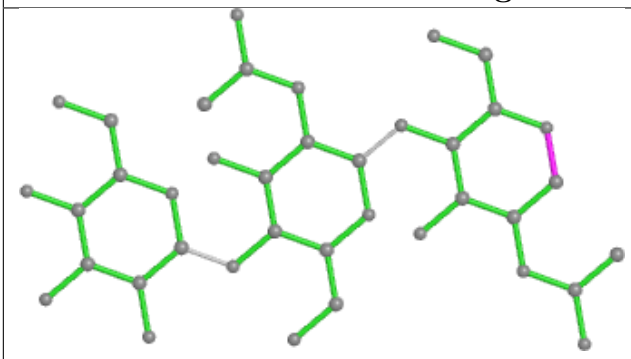
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	2	0
4	C	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

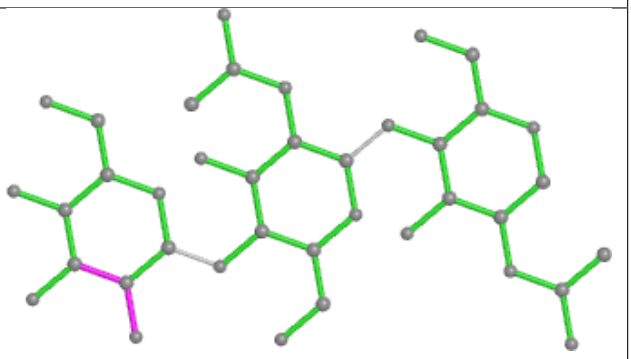
Oligosaccharide Chain E



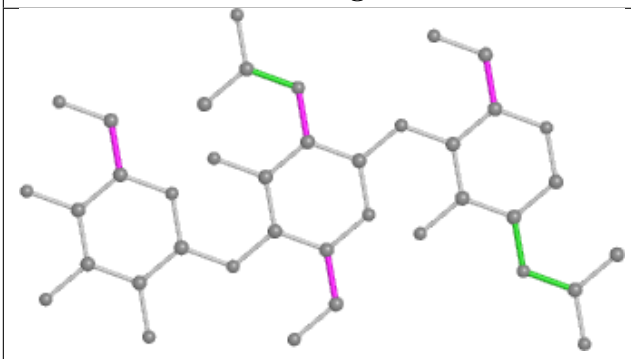
Oligosaccharide Chain C



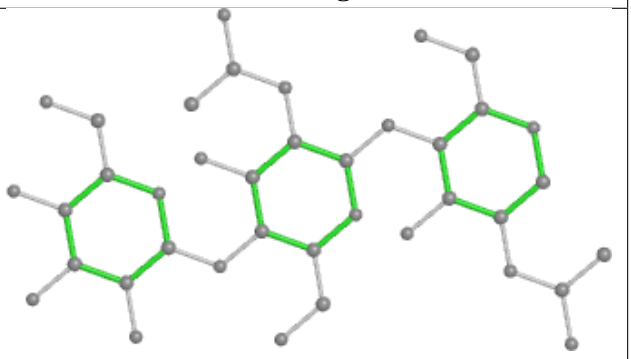
Bond lengths



Bond angles

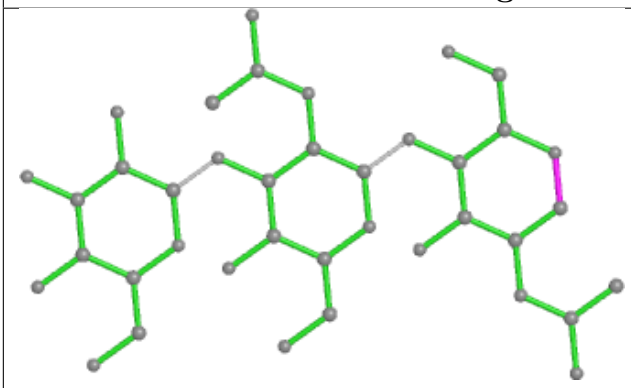


Torsions

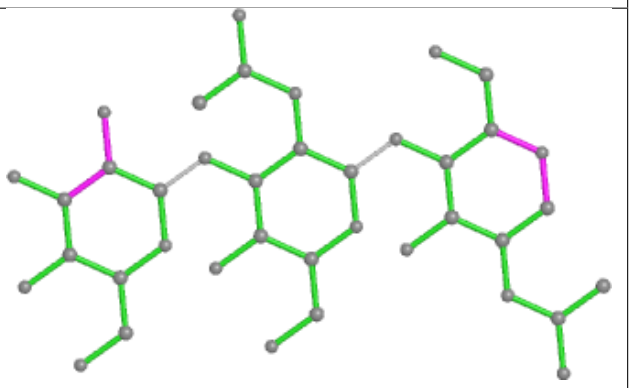


Rings

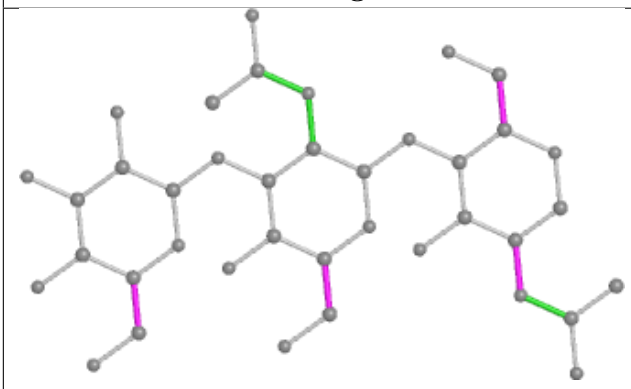
Oligosaccharide Chain F



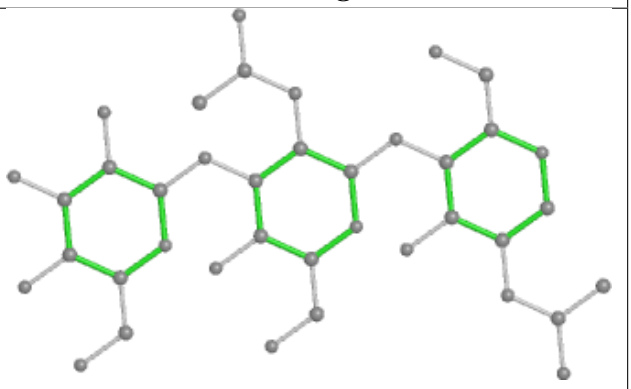
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 for Mogul analysis.

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	$\#\|Z\| > 2$
8	3PE	A	2404	-	39,39,50	0.30	0	42,44,55	0.37	0
11	NAG	D	1204	3	14,14,15	0.23	0	17,19,21	0.67	0
11	NAG	D	1203	3	14,14,15	0.45	0	17,19,21	0.47	0
11	NAG	D	1206	3	14,14,15	0.22	0	17,19,21	0.53	0
6	Y01	A	2401	-	38,38,38	0.43	0	57,57,57	0.47	0
6	Y01	A	2408	-	38,38,38	0.44	0	57,57,57	0.77	1 (1%)
11	NAG	D	1207	3	14,14,15	0.24	0	17,19,21	0.50	0
6	Y01	A	2414	-	38,38,38	0.45	0	57,57,57	0.74	0
6	Y01	A	2406	-	38,38,38	0.52	0	57,57,57	0.94	3 (5%)
7	R16	A	2407	-	15,15,15	0.20	0	14,14,14	0.17	0
7	R16	A	2409	-	12,12,15	0.17	0	11,11,14	0.13	0
6	Y01	A	2412	-	38,38,38	0.46	0	57,57,57	0.97	3 (5%)
11	NAG	D	1209	3	14,14,15	0.19	0	17,19,21	0.57	0
7	R16	A	2402	-	9,9,15	0.16	0	8,8,14	0.15	0
6	Y01	A	2411	-	38,38,38	0.43	0	57,57,57	0.80	3 (5%)
11	NAG	D	1202	3	14,14,15	0.17	0	17,19,21	0.47	0
11	NAG	D	1205	3	14,14,15	0.46	0	17,19,21	0.46	0
7	R16	A	2418	-	8,8,15	0.12	0	7,7,14	0.07	0
7	R16	A	2403	-	15,15,15	0.16	0	14,14,14	0.23	0
8	3PE	A	2405	-	39,39,50	0.30	0	42,44,55	0.37	0
7	R16	A	2419	-	15,15,15	0.09	0	14,14,14	0.20	0
11	NAG	D	1208	3	14,14,15	0.32	0	17,19,21	0.60	0
10	TOR	A	2416	-	24,24,24	12.63	19 (79%)	37,41,41	2.64	10 (27%)
6	Y01	A	2413	-	38,38,38	0.53	0	57,57,57	0.80	1 (1%)
6	Y01	A	2410	-	38,38,38	0.53	0	57,57,57	1.08	3 (5%)
6	Y01	A	2417	-	38,38,38	0.45	0	57,57,57	1.06	5 (8%)

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
8	3PE	A	2404	-	-	8/43/43/54	-
11	NAG	D	1204	3	-	2/6/23/26	0/1/1/1
11	NAG	D	1203	3	-	4/6/23/26	0/1/1/1
11	NAG	D	1206	3	-	0/6/23/26	0/1/1/1
6	Y01	A	2401	-	-	10/19/77/77	0/4/4/4
6	Y01	A	2408	-	-	9/19/77/77	0/4/4/4
11	NAG	D	1207	3	-	2/6/23/26	0/1/1/1
6	Y01	A	2414	-	-	15/19/77/77	0/4/4/4
6	Y01	A	2406	-	-	13/19/77/77	0/4/4/4
7	R16	A	2407	-	-	1/13/13/13	-
7	R16	A	2409	-	-	1/10/10/13	-
6	Y01	A	2412	-	-	8/19/77/77	0/4/4/4
11	NAG	D	1209	3	-	0/6/23/26	0/1/1/1
7	R16	A	2402	-	-	0/7/7/13	-
6	Y01	A	2411	-	-	9/19/77/77	0/4/4/4
11	NAG	D	1202	3	-	0/6/23/26	0/1/1/1
11	NAG	D	1205	3	-	4/6/23/26	0/1/1/1
7	R16	A	2418	-	-	0/6/6/13	-
7	R16	A	2403	-	-	3/13/13/13	-
8	3PE	A	2405	-	-	3/43/43/54	-
7	R16	A	2419	-	-	1/13/13/13	-
11	NAG	D	1208	3	-	3/6/23/26	0/1/1/1
10	TOR	A	2416	-	-	7/7/48/48	0/3/3/3
6	Y01	A	2413	-	-	13/19/77/77	0/4/4/4
6	Y01	A	2410	-	-	10/19/77/77	0/4/4/4
6	Y01	A	2417	-	-	12/19/77/77	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2416	TOR	OAI-SAO	28.50	1.65	1.42
10	A	2416	TOR	OAS-SAO	28.36	1.65	1.42
10	A	2416	TOR	CAL-CAK	-26.70	1.11	1.54
10	A	2416	TOR	OAQ-CAU	-17.01	1.10	1.43
10	A	2416	TOR	OAR-CAL	-14.39	1.16	1.42
10	A	2416	TOR	CAC-CAB	-13.26	1.29	1.51
10	A	2416	TOR	CAG-CAB	-12.57	1.19	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2416	TOR	SAO-NAP	11.03	1.70	1.58
10	A	2416	TOR	OAF-CAG	10.83	1.60	1.43
10	A	2416	TOR	OAA-CAB	9.28	1.64	1.43
10	A	2416	TOR	OAR-CAU	-9.02	1.30	1.44
10	A	2416	TOR	CAG-CAK	8.36	1.69	1.52
10	A	2416	TOR	OAA-CAE	-7.09	1.29	1.43
10	A	2416	TOR	OAH-CAL	-6.20	1.32	1.42
10	A	2416	TOR	OAN-SAO	6.05	1.66	1.57
10	A	2416	TOR	OAQ-CAK	-4.67	1.36	1.43
10	A	2416	TOR	OAH-CAC	4.48	1.50	1.43
10	A	2416	TOR	CAM-CAL	3.93	1.56	1.52
10	A	2416	TOR	OAN-CAM	-2.13	1.42	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2416	TOR	OAI-SAO-OAS	-10.24	110.28	119.97
10	A	2416	TOR	OAA-CAB-CAC	-5.45	100.26	110.45
10	A	2416	TOR	CAM-CAL-CAK	-5.43	103.84	115.42
10	A	2416	TOR	OAH-CAL-OAR	3.80	117.79	109.54
10	A	2416	TOR	CAU-OAQ-CAK	-3.77	101.46	108.73
6	A	2410	Y01	CAL-CAM-CAY	3.51	123.63	113.43
6	A	2410	Y01	CBI-CBE-CBB	3.45	124.88	119.49
6	A	2417	Y01	CAC-CBB-CBE	3.31	117.99	112.92
6	A	2417	Y01	CBI-CBE-CBB	3.24	124.56	119.49
10	A	2416	TOR	CAE-OAA-CAB	-3.17	102.97	108.19
6	A	2406	Y01	CAQ-CBG-CBI	3.13	107.62	103.84
10	A	2416	TOR	OAF-CAG-CAK	2.85	114.09	108.65
6	A	2412	Y01	CBH-CBF-CBD	-2.85	108.46	112.73
6	A	2410	Y01	CAP-CAQ-CBG	-2.69	99.80	105.13
10	A	2416	TOR	CAB-CAG-CAK	2.58	117.24	113.72
6	A	2412	Y01	CBF-CBD-CBG	2.56	112.52	109.09
6	A	2411	Y01	CAP-CBE-CBB	2.55	116.09	112.15
6	A	2417	Y01	CAP-CBE-CBI	-2.40	100.95	103.84
6	A	2408	Y01	CBH-CBF-CBD	-2.35	109.20	112.73
6	A	2406	Y01	CAU-CBI-CBG	-2.31	103.69	107.27
6	A	2411	Y01	CBG-CBI-CBE	-2.27	97.38	100.07
6	A	2406	Y01	CBI-CBG-CBD	-2.20	111.13	114.38
6	A	2413	Y01	CBH-CBF-CBD	-2.19	109.44	112.73
6	A	2417	Y01	CAL-CAM-CAY	2.18	119.77	113.43
6	A	2412	Y01	CAT-CAR-CBC	2.16	114.01	110.33
6	A	2417	Y01	CBH-CBF-CBD	-2.15	109.51	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2416	TOR	OAH-CAL-CAK	2.02	117.03	113.62
10	A	2416	TOR	CAU-OAR-CAL	-2.00	107.69	109.68
6	A	2411	Y01	CBI-CBE-CBB	2.00	122.62	119.49

There are no chirality outliers.

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2401	Y01	OAG-CAY-OAW-CBC
6	A	2401	Y01	CAM-CAY-OAW-CBC
6	A	2406	Y01	CAR-CBC-OAW-CAY
6	A	2406	Y01	CAM-CAY-OAW-CBC
6	A	2410	Y01	CAO-CBB-CBE-CBI
6	A	2410	Y01	CAR-CBC-OAW-CAY
6	A	2411	Y01	CAR-CBC-OAW-CAY
6	A	2413	Y01	CAO-CBB-CBE-CAP
6	A	2413	Y01	CAC-CBB-CBE-CBI
6	A	2413	Y01	OAG-CAY-OAW-CBC
6	A	2414	Y01	CAO-CBB-CBE-CAP
6	A	2414	Y01	CAO-CBB-CBE-CBI
6	A	2414	Y01	CAC-CBB-CBE-CBI
6	A	2417	Y01	OAG-CAY-OAW-CBC
6	A	2417	Y01	CAM-CAY-OAW-CBC
10	A	2416	TOR	OAR-CAL-CAM-OAN
10	A	2416	TOR	CAL-CAM-OAN-SAO
10	A	2416	TOR	CAM-OAN-SAO-OAS
10	A	2416	TOR	CAM-OAN-SAO-OAI
10	A	2416	TOR	CAM-OAN-SAO-NAP
11	D	1203	NAG	C1-C2-N2-C7
6	A	2413	Y01	CAC-CBB-CBE-CAP
6	A	2414	Y01	CAC-CBB-CBE-CAP
6	A	2417	Y01	CAC-CBB-CBE-CAP
6	A	2417	Y01	CAC-CBB-CBE-CBI
6	A	2417	Y01	CAO-CBB-CBE-CAP
6	A	2413	Y01	CAO-CBB-CBE-CBI
6	A	2406	Y01	OAG-CAY-OAW-CBC
11	D	1208	NAG	C4-C5-C6-O6
6	A	2413	Y01	CAM-CAY-OAW-CBC
6	A	2406	Y01	CAJ-CAO-CBB-CAC
6	A	2417	Y01	CAO-CBB-CBE-CBI
11	D	1208	NAG	O5-C5-C6-O6
11	D	1203	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	D	1207	NAG	O5-C5-C6-O6
6	A	2406	Y01	CAJ-CAO-CBB-CBE
6	A	2401	Y01	CAJ-CAO-CBB-CAC
6	A	2413	Y01	CAJ-CAO-CBB-CAC
6	A	2401	Y01	CAJ-CAO-CBB-CBE
6	A	2412	Y01	CAJ-CAO-CBB-CBE
6	A	2410	Y01	CAC-CBB-CBE-CAP
6	A	2410	Y01	CAO-CBB-CBE-CAP
6	A	2401	Y01	CAO-CBB-CBE-CBI
6	A	2411	Y01	CAO-CBB-CBE-CBI
6	A	2413	Y01	CAJ-CAO-CBB-CBE
11	D	1205	NAG	O5-C5-C6-O6
11	D	1207	NAG	C4-C5-C6-O6
6	A	2412	Y01	CAJ-CAO-CBB-CAC
6	A	2411	Y01	CAC-CBB-CBE-CAP
6	A	2401	Y01	CAC-CBB-CBE-CAP
6	A	2401	Y01	CAC-CBB-CBE-CBI
11	D	1203	NAG	O5-C5-C6-O6
11	D	1205	NAG	C1-C2-N2-C7
6	A	2408	Y01	CAN-CAJ-CAO-CBB
6	A	2411	Y01	CAC-CBB-CBE-CBI
6	A	2406	Y01	CAN-CAJ-CAO-CBB
8	A	2404	3PE	C1-O11-P-O13
6	A	2413	Y01	CAJ-CAN-CBA-CAB
6	A	2411	Y01	CAM-CAY-OAW-CBC
6	A	2410	Y01	CAC-CBB-CBE-CBI
6	A	2414	Y01	CAJ-CAN-CBA-CAA
6	A	2411	Y01	CAN-CAJ-CAO-CBB
6	A	2413	Y01	CAO-CAJ-CAN-CBA
11	D	1205	NAG	C4-C5-C6-O6
6	A	2411	Y01	OAG-CAY-OAW-CBC
6	A	2408	Y01	CAM-CAY-OAW-CBC
6	A	2413	Y01	CAJ-CAN-CBA-CAA
8	A	2404	3PE	C22-C21-O21-C2
6	A	2406	Y01	CAJ-CAN-CBA-CAB
6	A	2408	Y01	OAG-CAY-OAW-CBC
10	A	2416	TOR	OAH-CAL-CAM-OAN
8	A	2404	3PE	O22-C21-O21-C2
6	A	2414	Y01	CAJ-CAN-CBA-CAB
6	A	2417	Y01	CAN-CAJ-CAO-CBB
7	A	2403	R16	C28-C29-C30-C31
6	A	2414	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
6	A	2408	Y01	CAC-CBB-CBE-CBI
6	A	2401	Y01	CAO-CBB-CBE-CAP
6	A	2408	Y01	CAO-CBB-CBE-CBI
6	A	2414	Y01	CAM-CAY-OAW-CBC
8	A	2404	3PE	C1-C2-C3-O31
6	A	2406	Y01	CAO-CAJ-CAN-CBA
6	A	2406	Y01	CAJ-CAN-CBA-CAA
6	A	2410	Y01	CAL-CAM-CAY-OAW
8	A	2404	3PE	C2-C1-O11-P
7	A	2403	R16	C33-C34-C35-C36
6	A	2412	Y01	CAJ-CAN-CBA-CAB
8	A	2404	3PE	O21-C2-C3-O31
6	A	2412	Y01	CAM-CAY-OAW-CBC
6	A	2414	Y01	OAG-CAY-OAW-CBC
8	A	2404	3PE	C1-O11-P-O14
6	A	2417	Y01	CAJ-CAN-CBA-CAB
7	A	2403	R16	C38-C39-C40-C41
6	A	2408	Y01	CAO-CBB-CBE-CAP
6	A	2412	Y01	OAG-CAY-OAW-CBC
6	A	2410	Y01	CAV-CBC-OAW-CAY
8	A	2405	3PE	C1-O11-P-O13
11	D	1203	NAG	C3-C2-N2-C7
11	D	1204	NAG	C3-C2-N2-C7
11	D	1205	NAG	C3-C2-N2-C7
11	D	1208	NAG	C3-C2-N2-C7
6	A	2414	Y01	CAJ-CAO-CBB-CBE
6	A	2406	Y01	CAX-CAL-CAM-CAY
6	A	2408	Y01	CAM-CAL-CAX-OAF
6	A	2414	Y01	CAJ-CAO-CBB-CAC
6	A	2408	Y01	CAC-CBB-CBE-CAP
7	A	2419	R16	C30-C31-C32-C33
11	D	1204	NAG	C1-C2-N2-C7
6	A	2401	Y01	CAM-CAL-CAX-OAF
6	A	2408	Y01	CAM-CAL-CAX-OAH
6	A	2406	Y01	CAV-CBC-OAW-CAY
6	A	2413	Y01	CAM-CAL-CAX-OAH
8	A	2404	3PE	C36-C37-C38-C39
6	A	2401	Y01	CAM-CAL-CAX-OAH
6	A	2417	Y01	CAJ-CAO-CBB-CBE
6	A	2410	Y01	CAM-CAL-CAX-OAH
6	A	2412	Y01	CAM-CAL-CAX-OAH
6	A	2414	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
6	A	2414	Y01	CAV-CBC-OAW-CAY
6	A	2417	Y01	CAM-CAL-CAX-OAH
6	A	2406	Y01	CAM-CAL-CAX-OAH
6	A	2414	Y01	CAR-CBC-OAW-CAY
6	A	2410	Y01	CAM-CAL-CAX-OAF
6	A	2413	Y01	CAM-CAL-CAX-OAF
7	A	2409	R16	C30-C31-C32-C33
7	A	2407	R16	C39-C40-C41-C42
6	A	2417	Y01	CAJ-CAN-CBA-CAA
6	A	2417	Y01	CAM-CAL-CAX-OAF
6	A	2406	Y01	CAM-CAL-CAX-OAF
6	A	2414	Y01	CAM-CAL-CAX-OAF
10	A	2416	TOR	CAK-CAL-CAM-OAN
6	A	2410	Y01	CAL-CAM-CAY-OAG
6	A	2411	Y01	CAM-CAL-CAX-OAH
6	A	2412	Y01	CAM-CAL-CAX-OAF
8	A	2405	3PE	C1-O11-P-O14
6	A	2412	Y01	CAJ-CAN-CBA-CAA
6	A	2411	Y01	CAM-CAL-CAX-OAF
8	A	2405	3PE	O31-C31-C32-C33

There are no ring outliers.

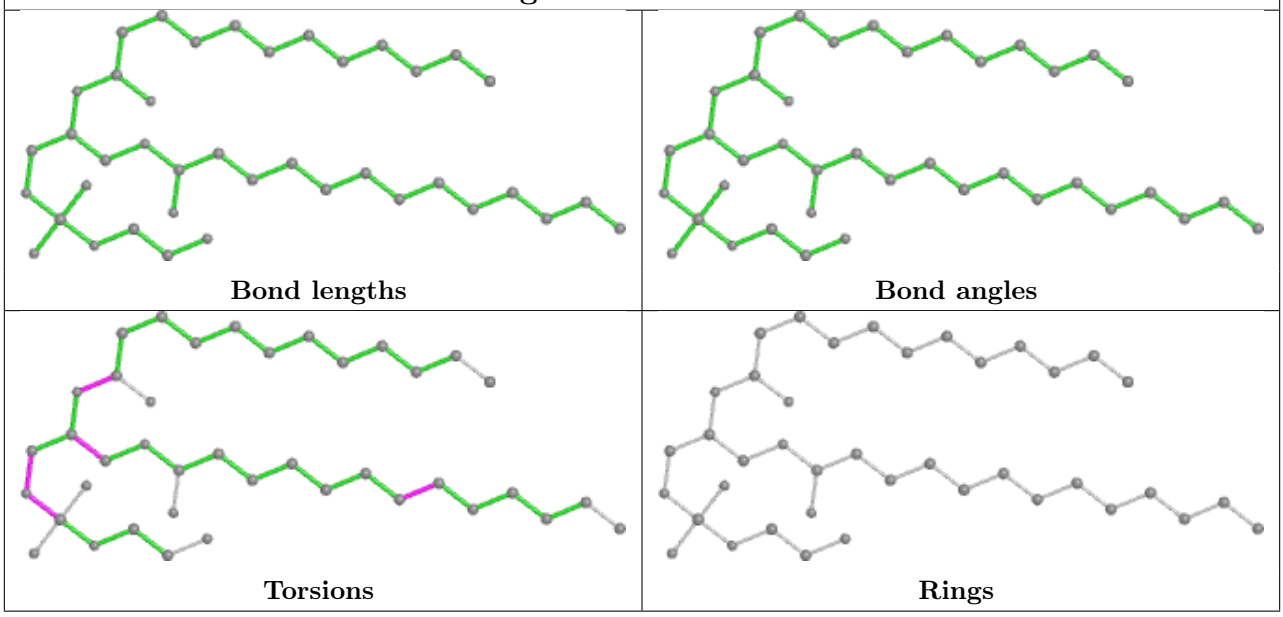
15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1203	NAG	1	0
6	A	2401	Y01	6	0
6	A	2408	Y01	2	0
6	A	2414	Y01	1	0
6	A	2406	Y01	7	0
7	A	2407	R16	1	0
7	A	2409	R16	1	0
6	A	2412	Y01	6	0
6	A	2411	Y01	2	0
11	D	1205	NAG	1	0
7	A	2419	R16	1	0
10	A	2416	TOR	5	0
6	A	2413	Y01	4	0
6	A	2410	Y01	6	0
6	A	2417	Y01	5	0

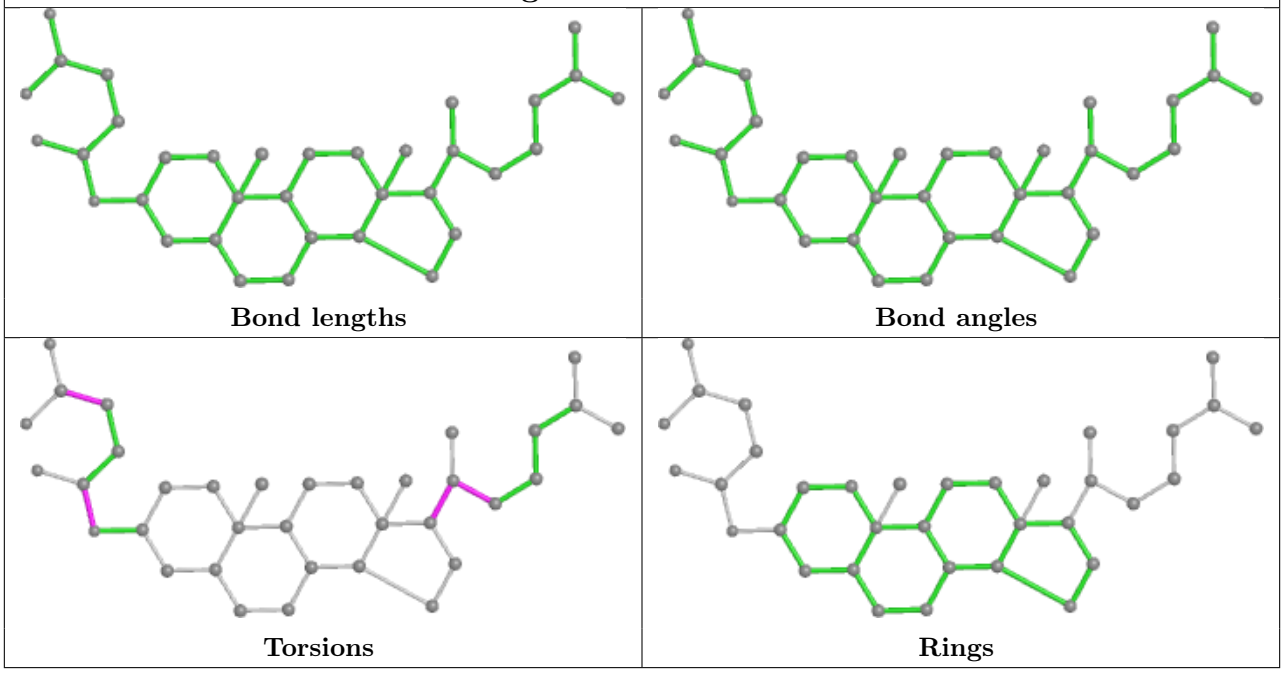
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

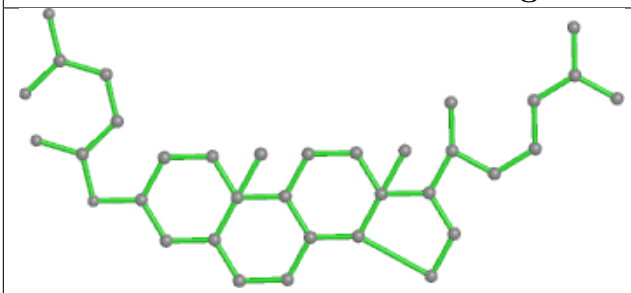
Ligand 3PE A 2404



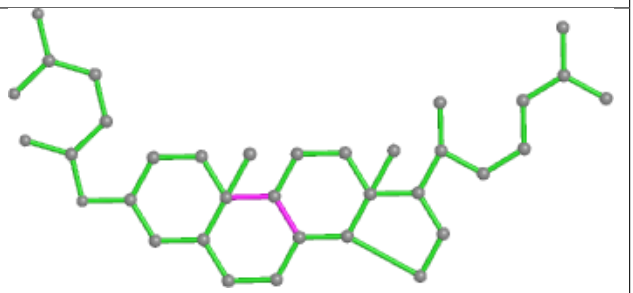
Ligand Y01 A 2401



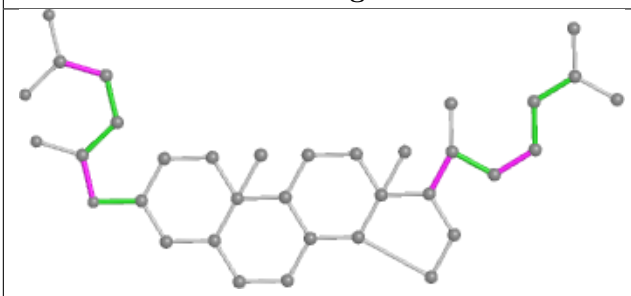
Ligand Y01 A 2408



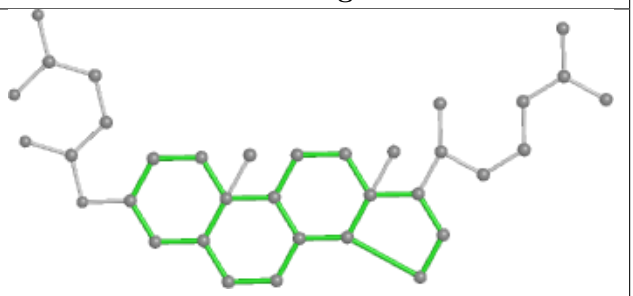
Bond lengths



Bond angles

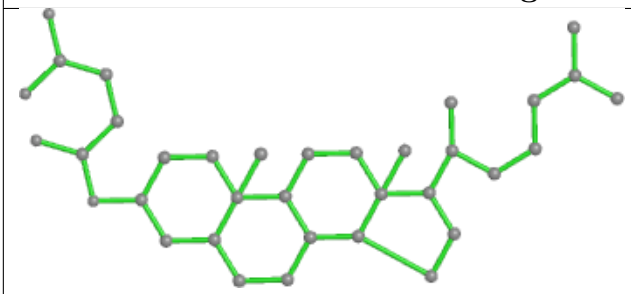


Torsions

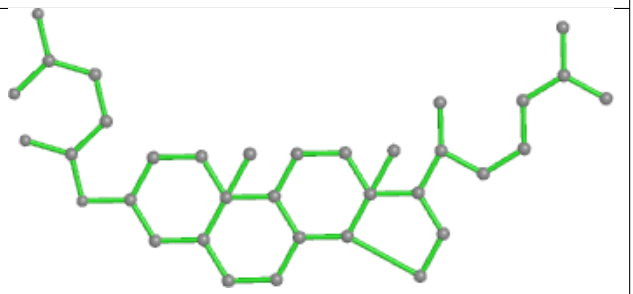


Rings

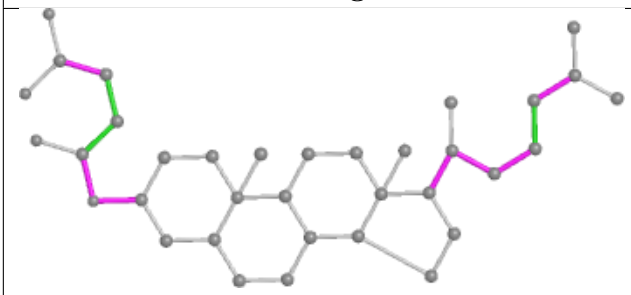
Ligand Y01 A 2414



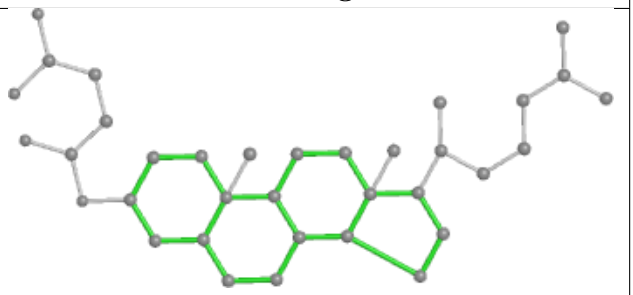
Bond lengths



Bond angles

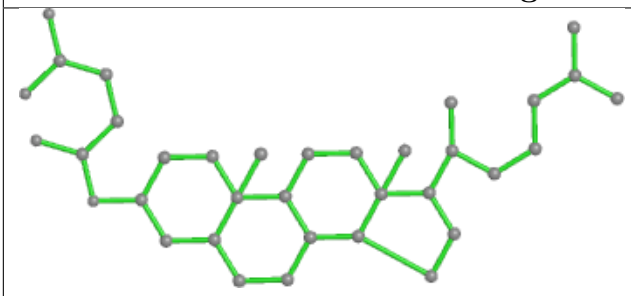


Torsions

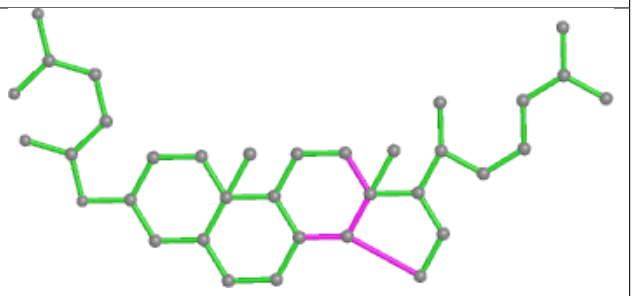


Rings

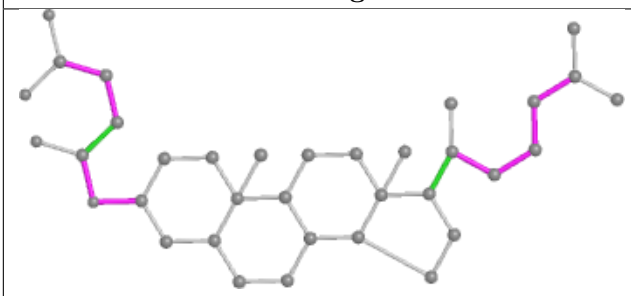
Ligand Y01 A 2406



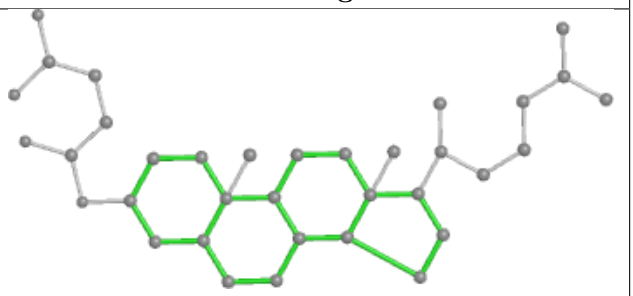
Bond lengths



Bond angles

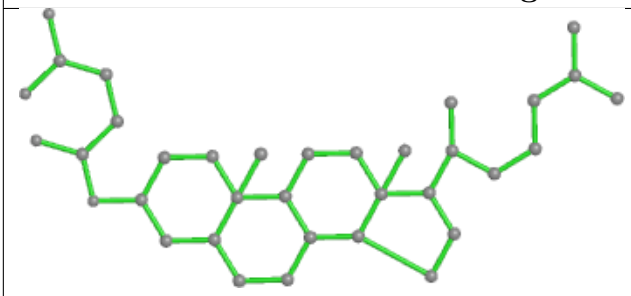


Torsions

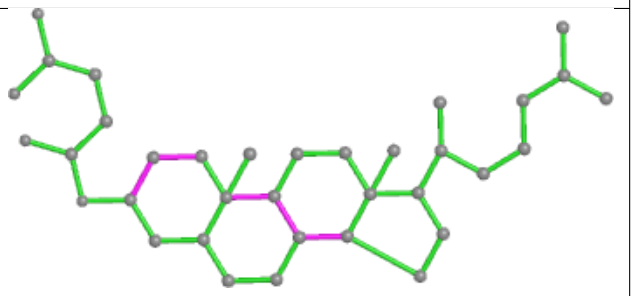


Rings

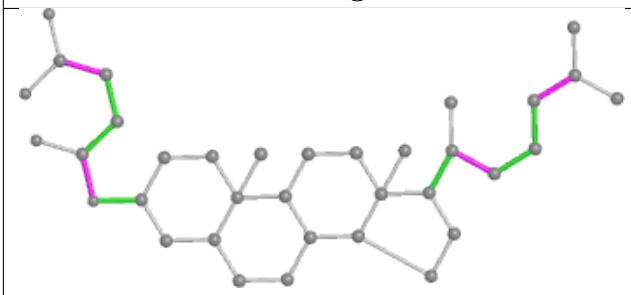
Ligand Y01 A 2412



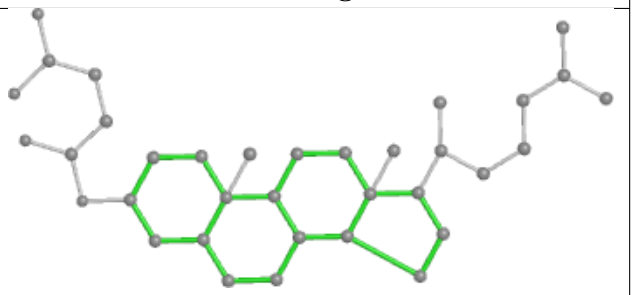
Bond lengths



Bond angles

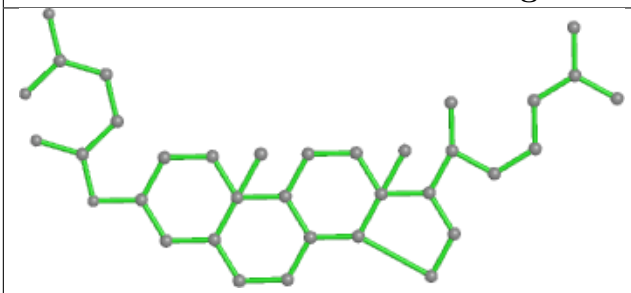


Torsions

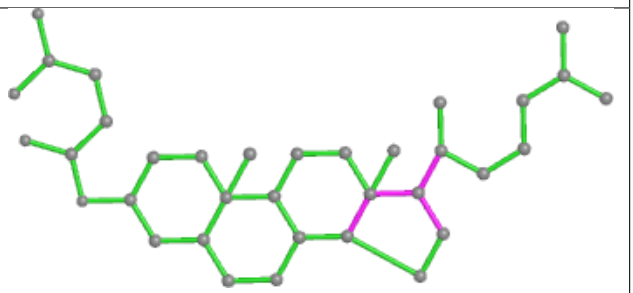


Rings

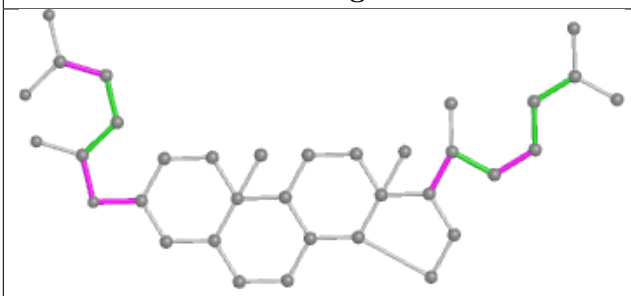
Ligand Y01 A 2411



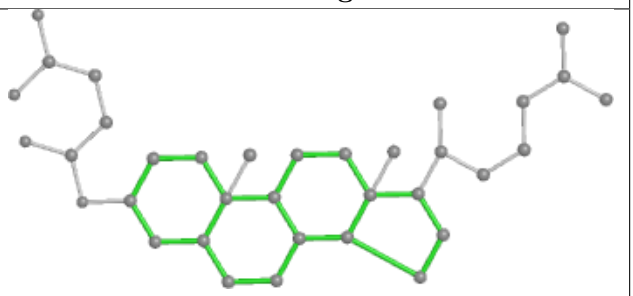
Bond lengths



Bond angles

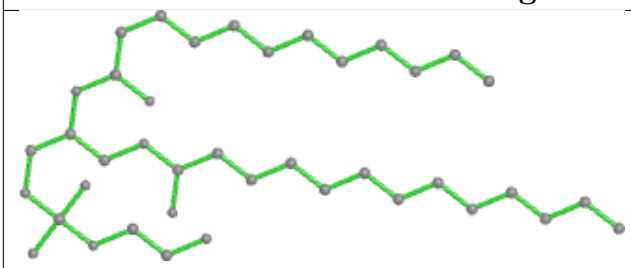


Torsions

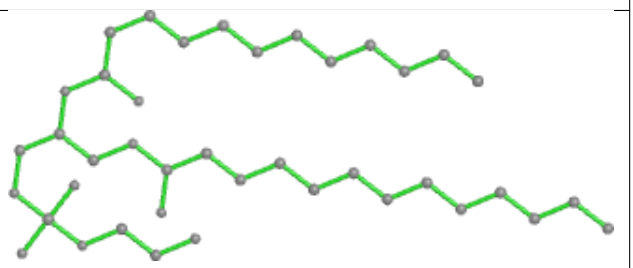


Rings

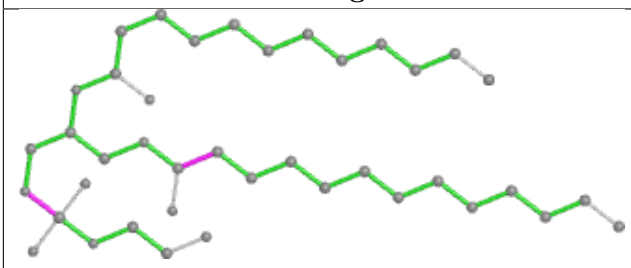
Ligand 3PE A 2405



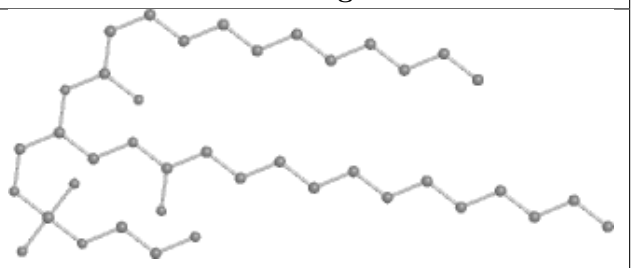
Bond lengths



Bond angles

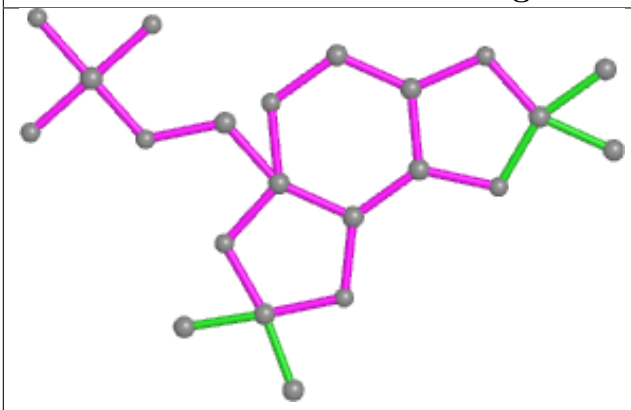


Torsions

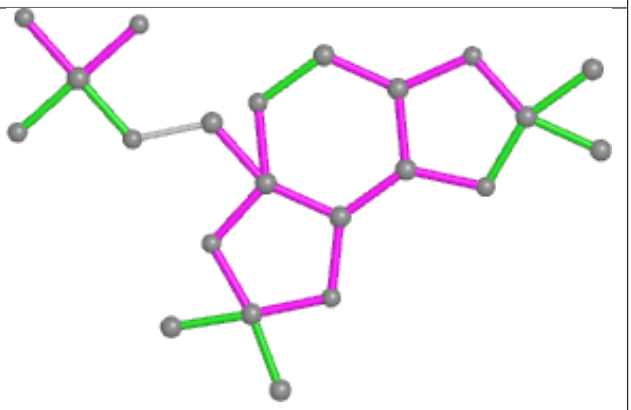


Rings

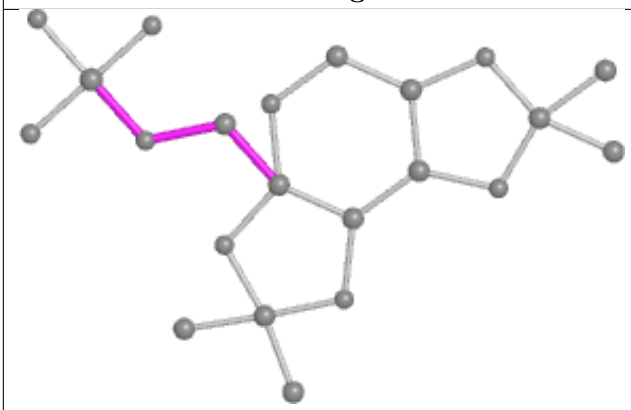
Ligand TOR A 2416



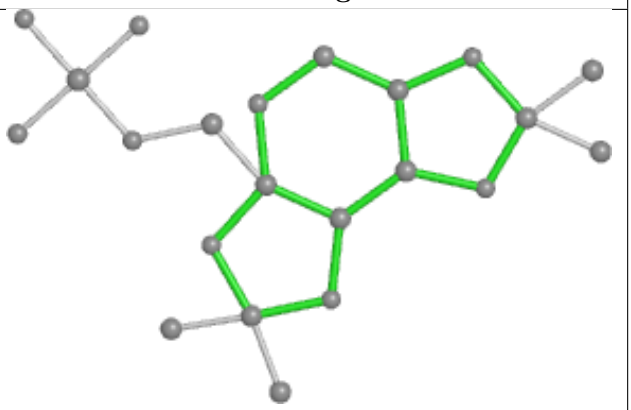
Bond lengths



Bond angles

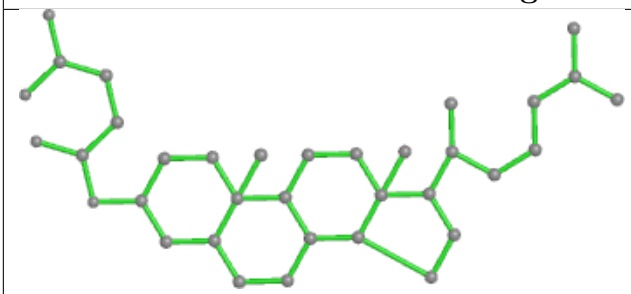


Torsions

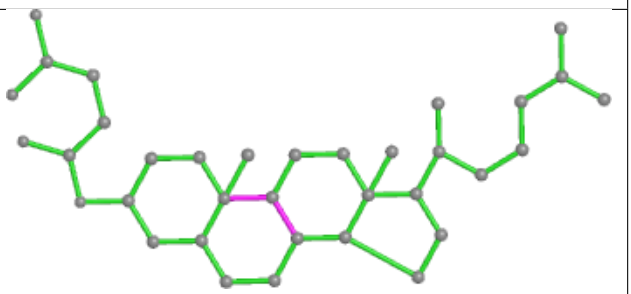


Rings

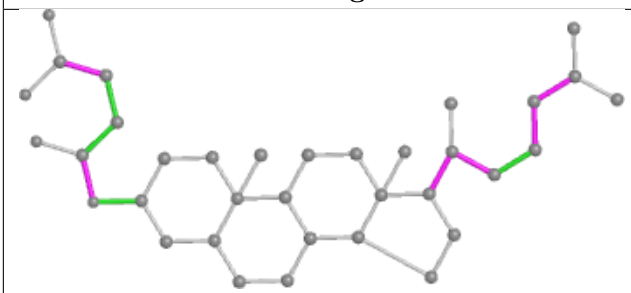
Ligand Y01 A 2413



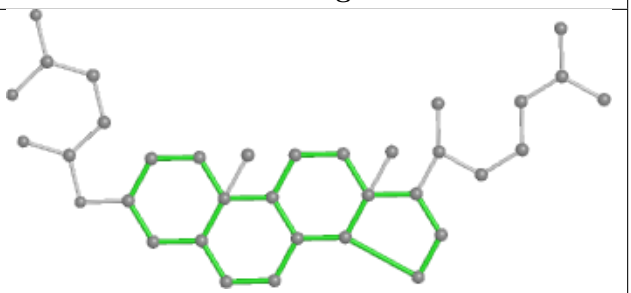
Bond lengths



Bond angles

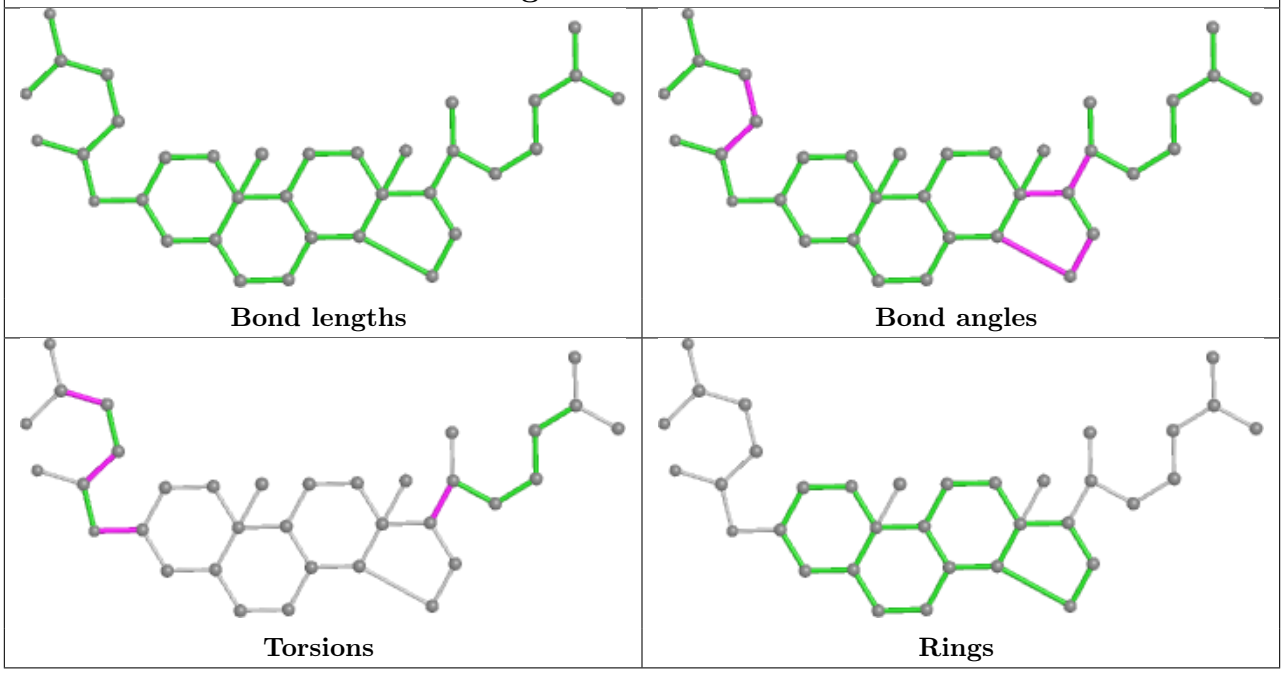


Torsions

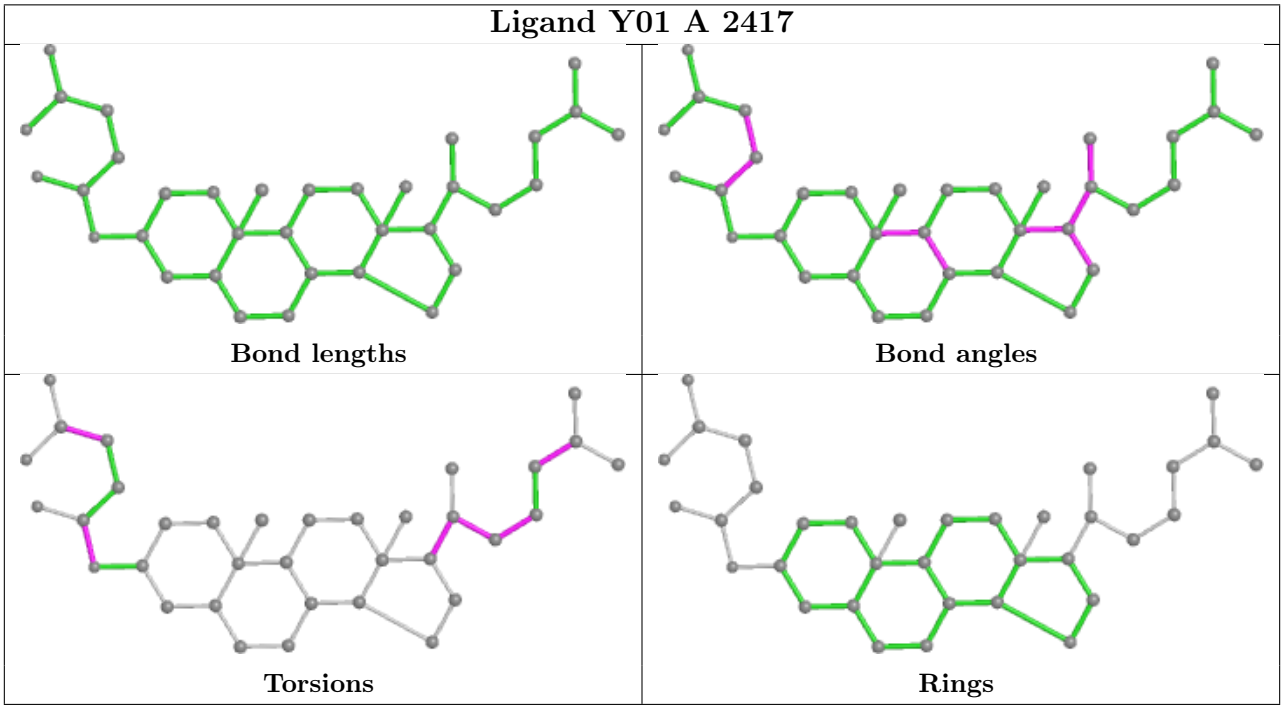


Rings

Ligand Y01 A 2410



Ligand Y01 A 2417



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.

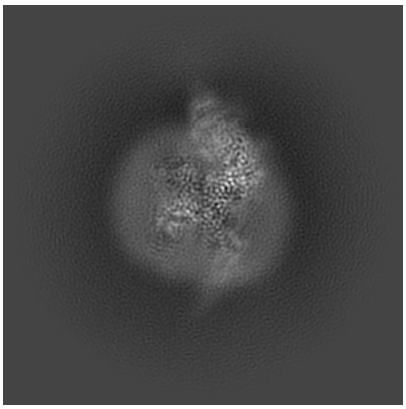
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33808. These allow visual inspection of the internal detail of the map and identification of artifacts.

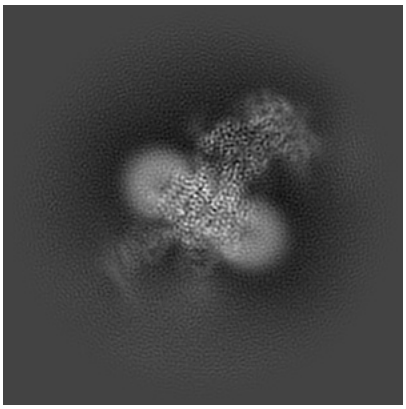
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

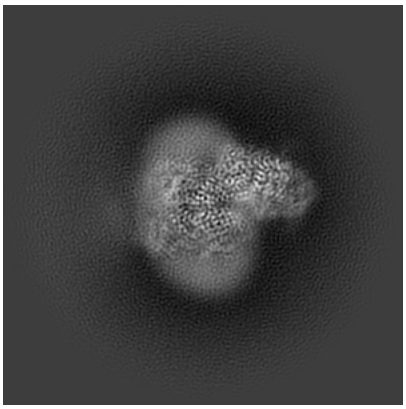
6.1.1 Primary map



X

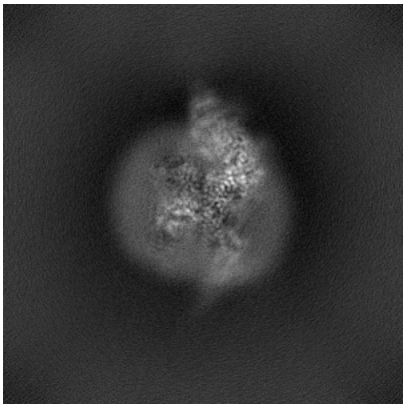


Y

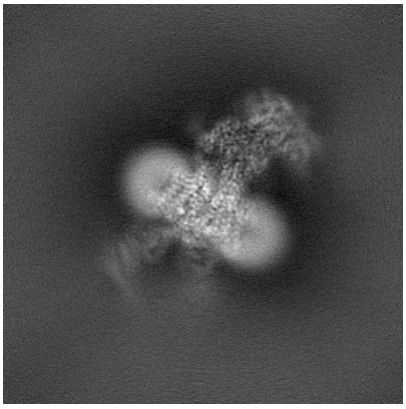


Z

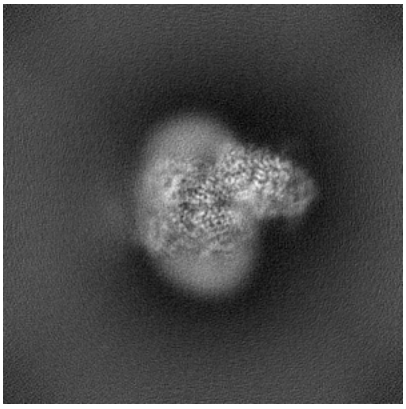
6.1.2 Raw map



X



Y

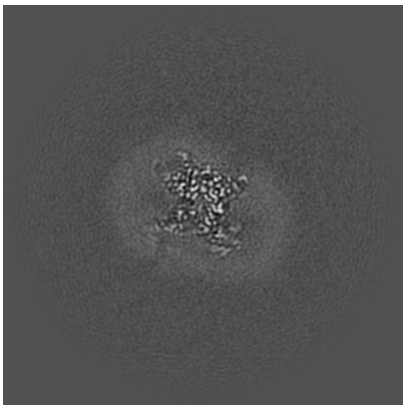


Z

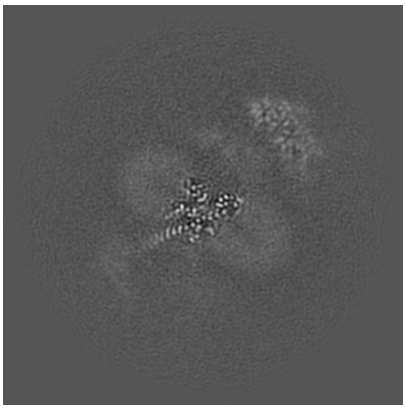
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

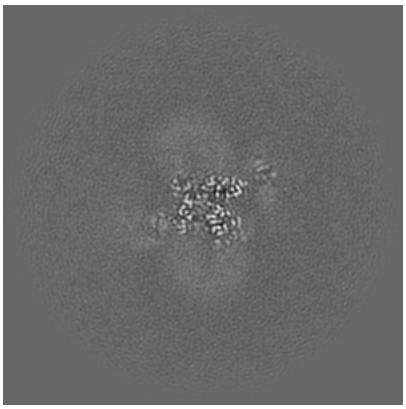
6.2.1 Primary map



X Index: 160

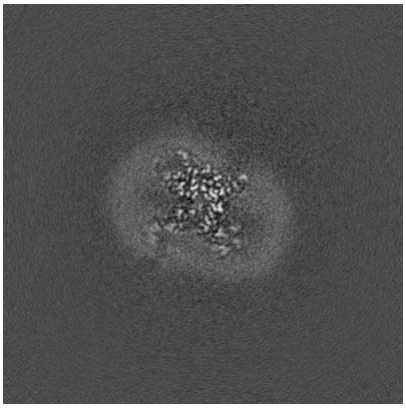


Y Index: 160

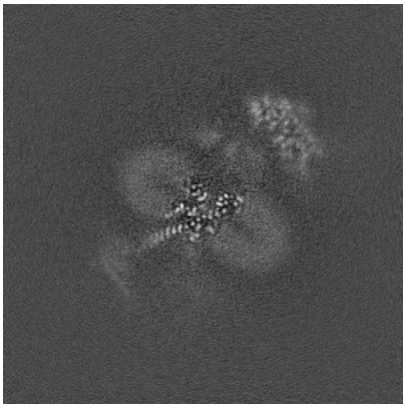


Z Index: 160

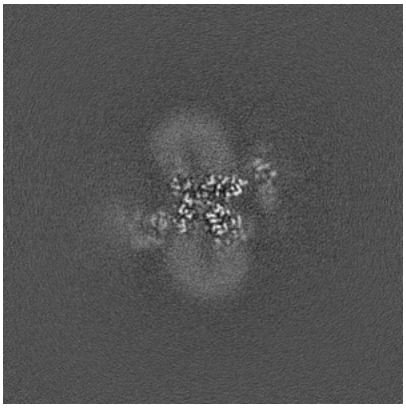
6.2.2 Raw map



X Index: 160



Y Index: 160

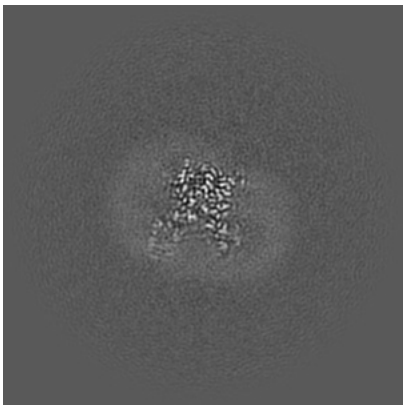


Z Index: 160

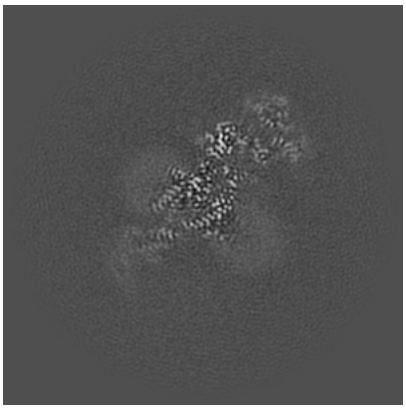
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

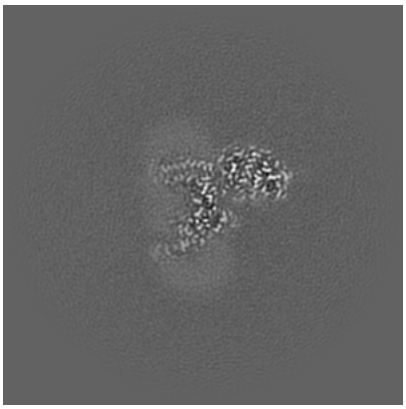
6.3.1 Primary map



X Index: 163

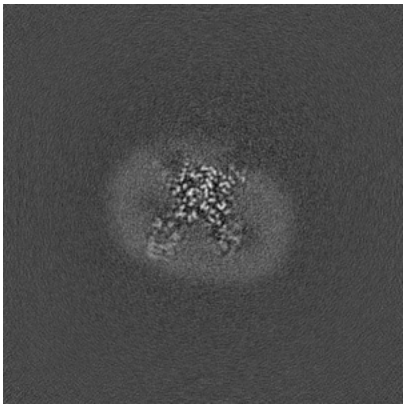


Y Index: 175

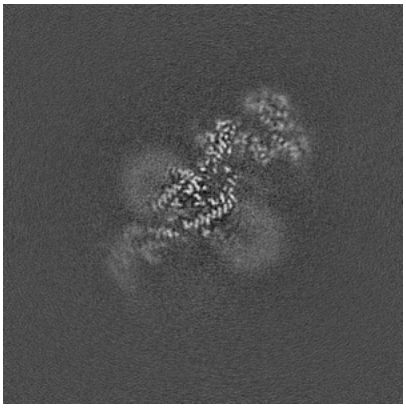


Z Index: 180

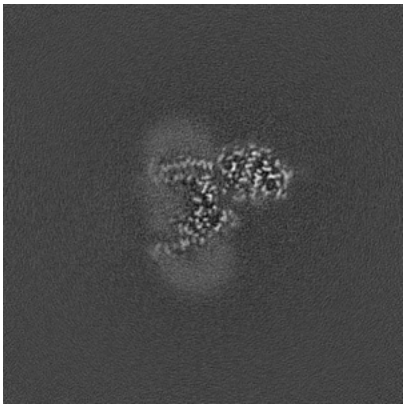
6.3.2 Raw map



X Index: 164



Y Index: 174

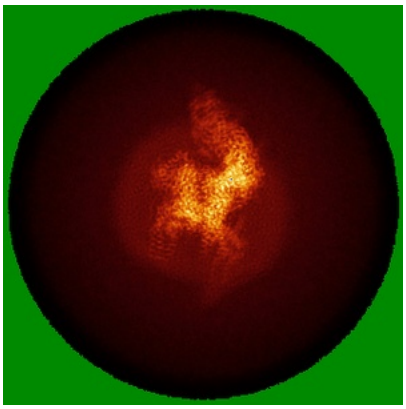


Z Index: 180

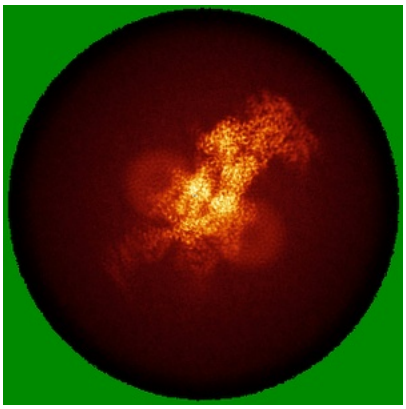
The images above show the largest variance slices of the map in three orthogonal directions.

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

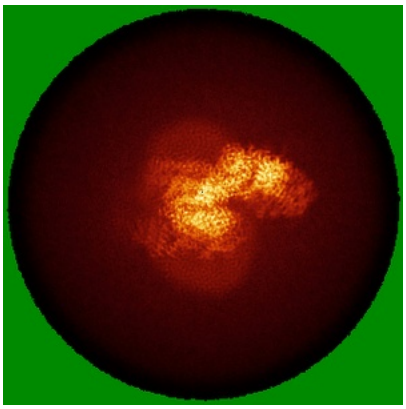
6.4.1 Primary map



X

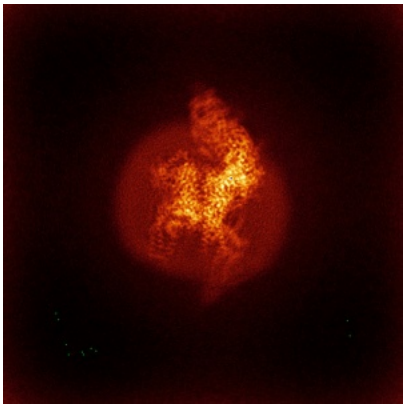


Y

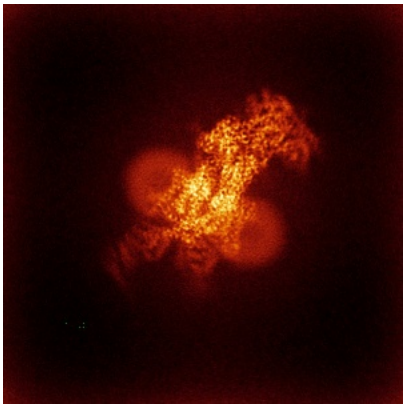


Z

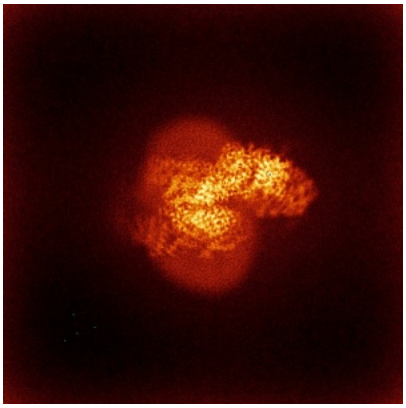
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

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

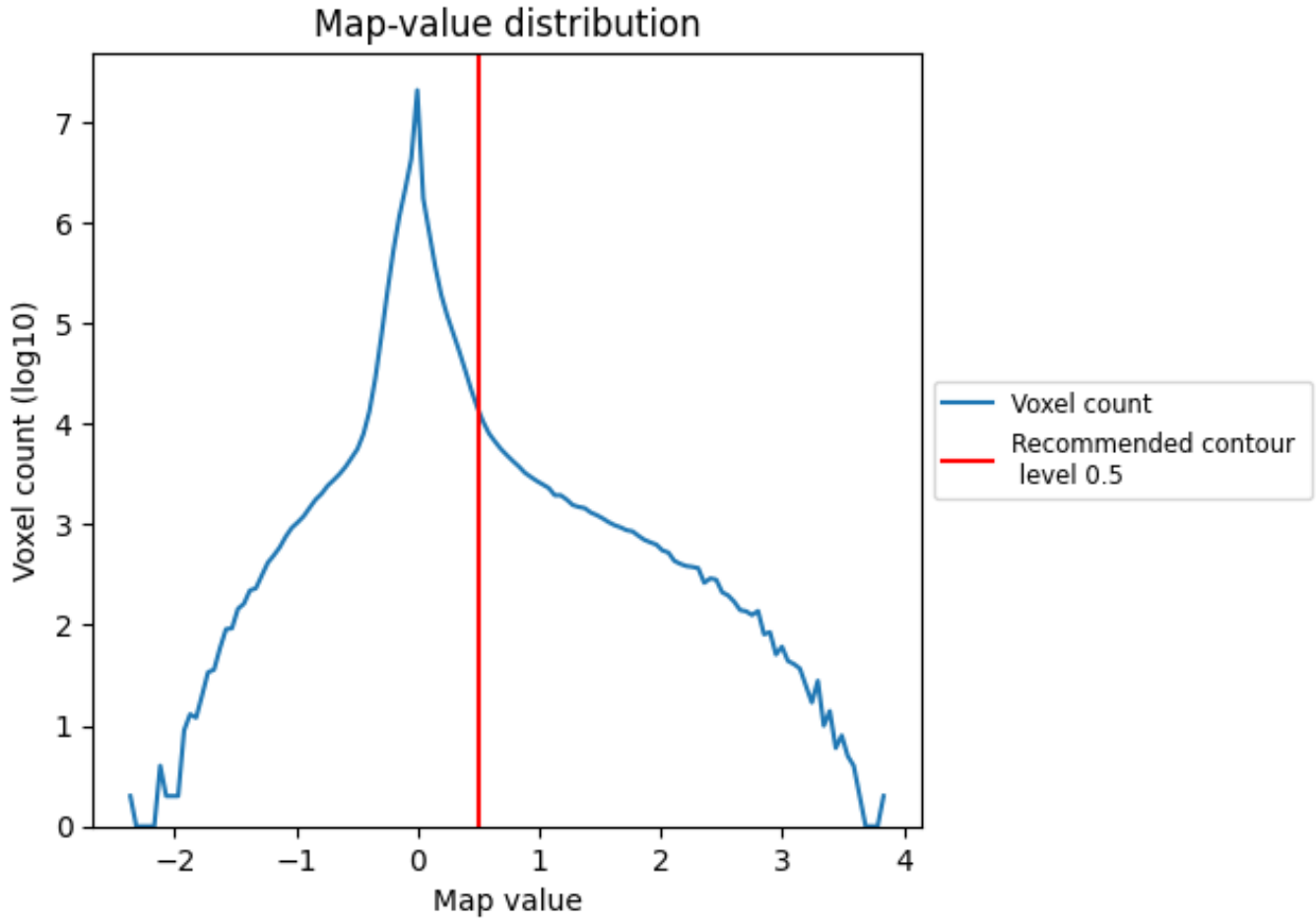
6.6 Mask visualisation (i)

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

7 Map analysis

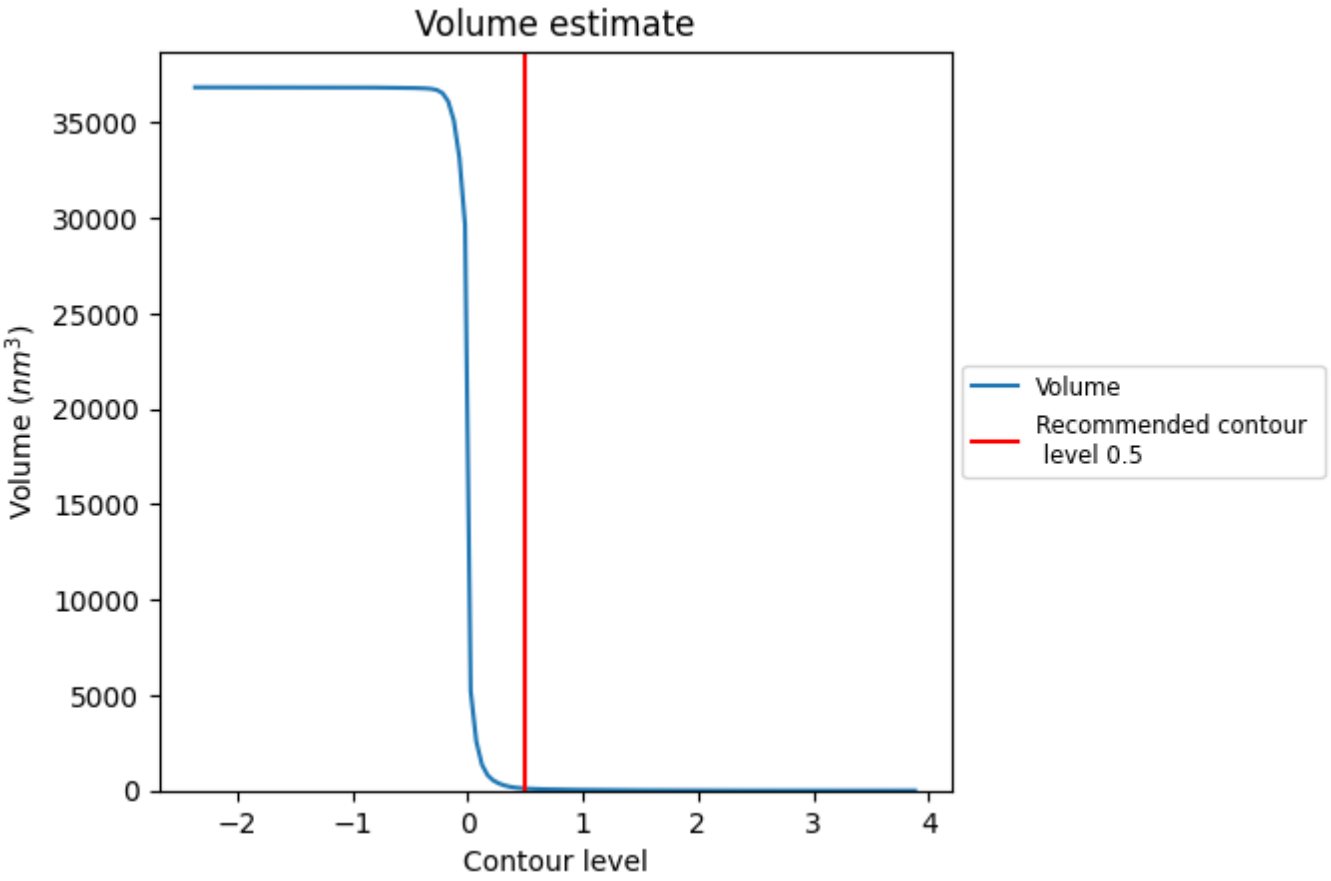
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

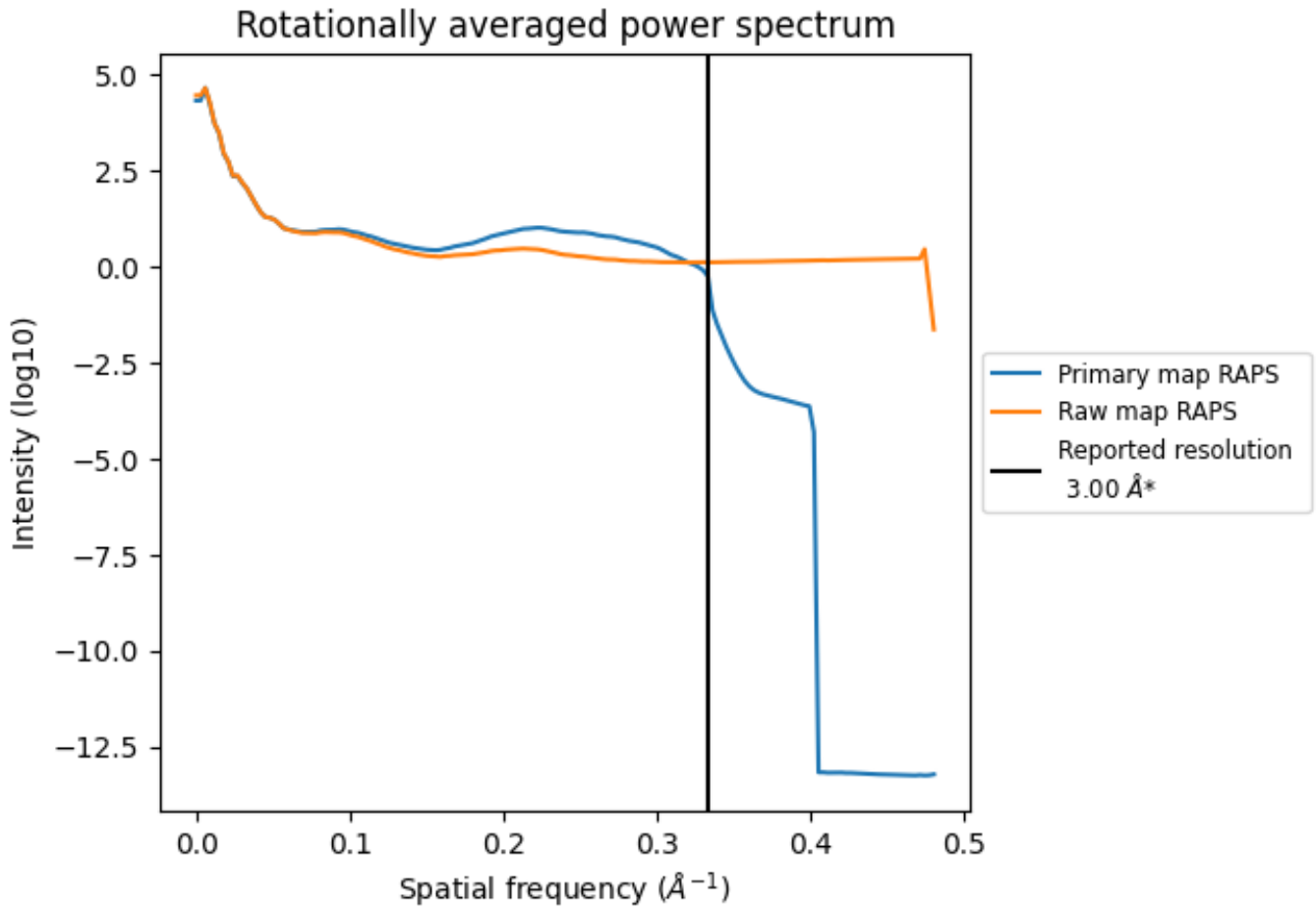
7.2 Volume estimate



The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 98 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)

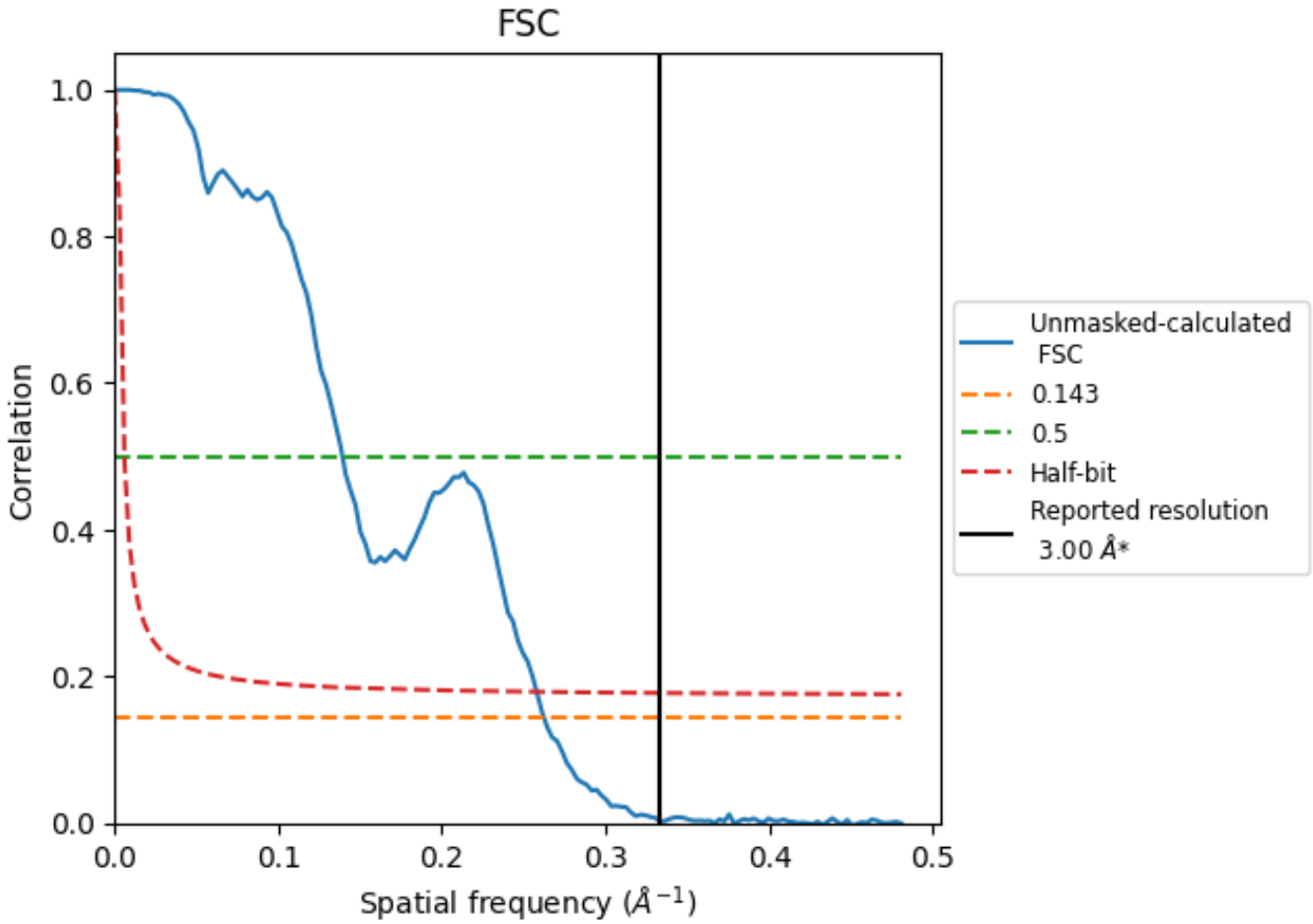


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

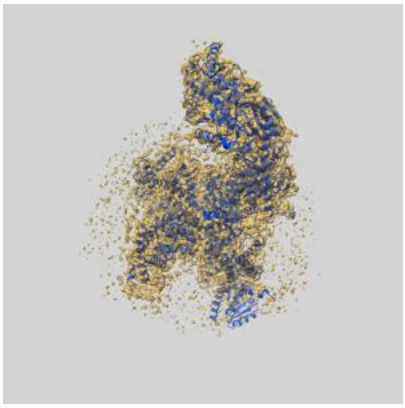
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	7.18	3.88

*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 3.81 differs from the reported value 3.0 by more than 10 %

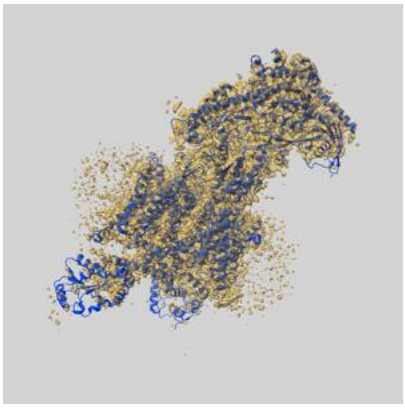
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33808 and PDB model 7YG5. Per-residue inclusion information can be found in section 3 on page 9.

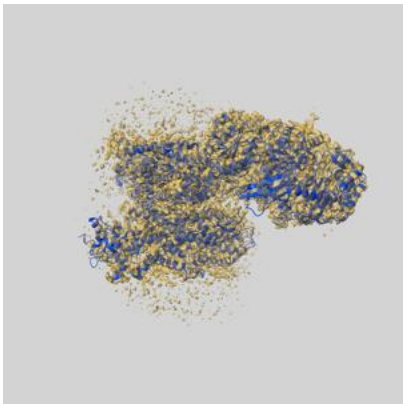
9.1 Map-model overlay



X



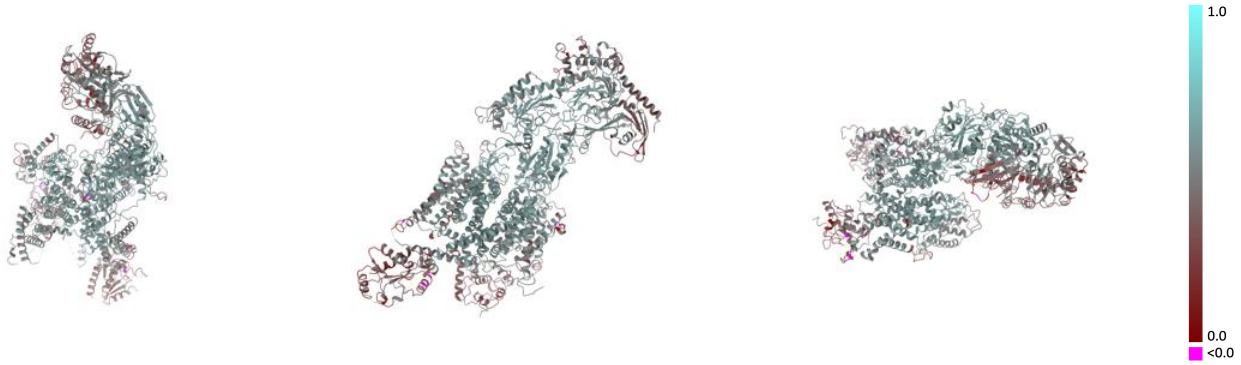
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

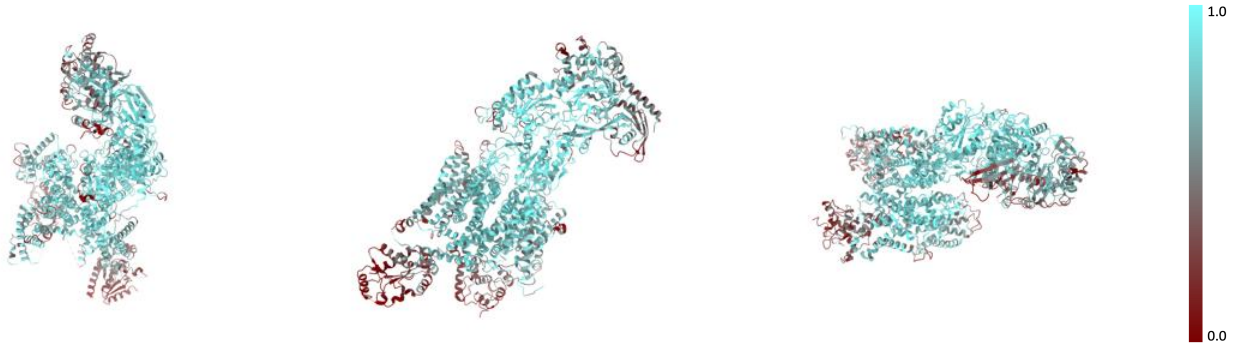
9.2 Q-score mapped to coordinate model (i)



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.

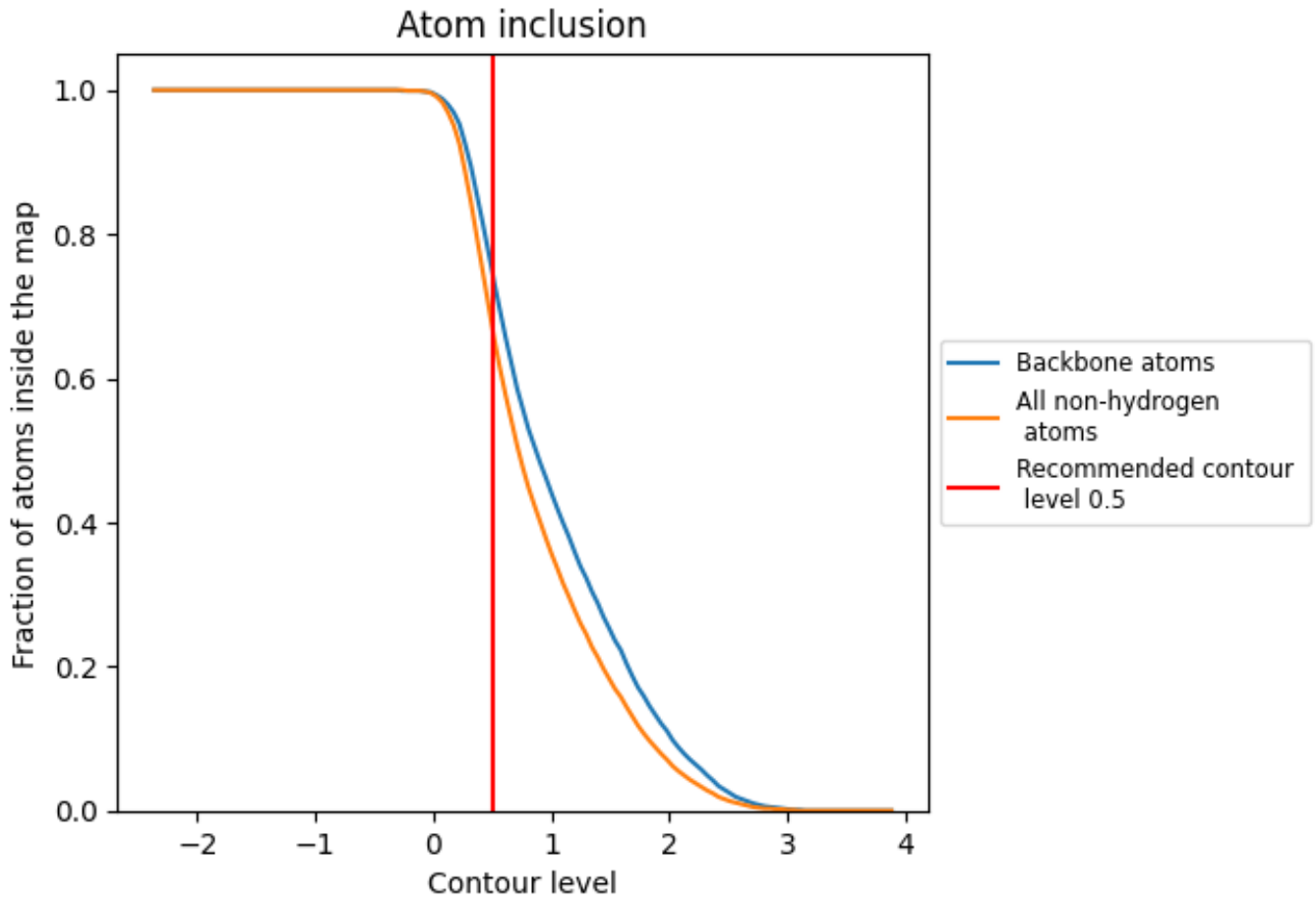
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.4910
A	0.6960	0.5030
B	0.2200	0.3230
C	0.8720	0.5560
D	0.7140	0.5040
E	0.4620	0.4030
F	0.1790	0.3500