Full wwPDB EM Validation Report ⓘ

Nov 28, 2023 – 06:22 PM JST

PDB ID	:	8WE9
EMDB ID	:	EMD-37475
Title	:	Human L-type voltage-gated calcium channel Cav1.2 (Class I) in the presence of pinaverium at 3.0 Angstrom resolution
Authors	:	Gao, S.; Yao, X.; Fan, X.; Yan, N.
Deposited on	:	2023-09-17
Resolution	:	3.00 Å(reported)

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:

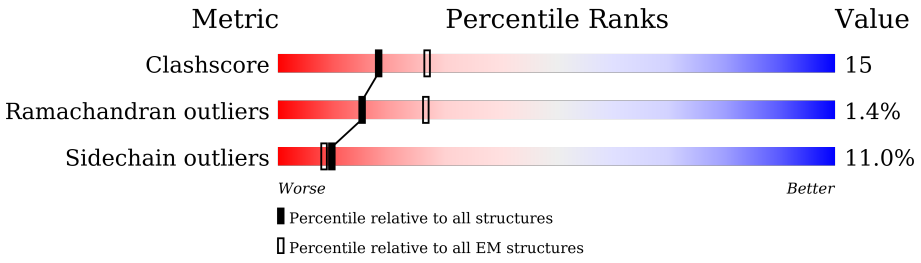
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2201	7%, 39%, 15%, ·, 43%
2	D	1103	·, 61%, 23%, ·, 14%
3	C	484	62%, 37%, 25%, 5%, 33%
4	B	3	33%, 67%, 33%
5	E	2	50%, 100%
5	G	2	50%, 100%
5	H	2	100%
6	F	4	25%, 25%, 25%, 50%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 20730 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 L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1260	10172	6686	1659	1764	63	0	0

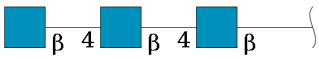
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	948	7570	4803	1269	1467	31	0	0

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	324	2575	1619	467	479	10	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	B	3	42	24	3	15	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
5	E	2	Total C N O 28 16 2 10	0	0
5	G	2	Total C N O 28 16 2 10	0	0
5	H	2	Total C N O 28 16 2 10	0	0

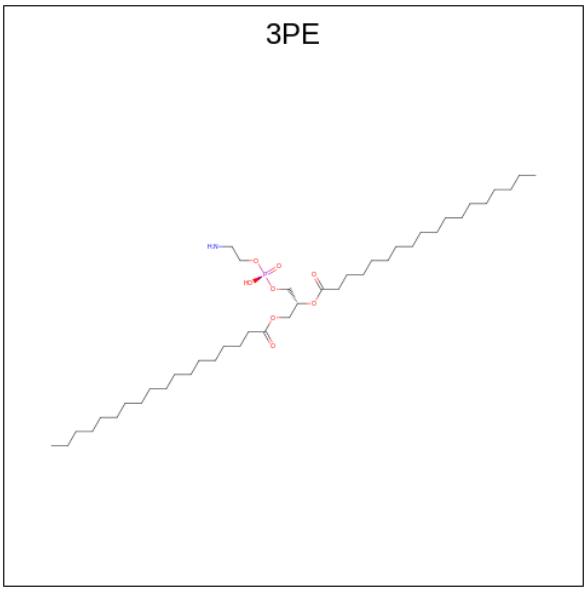
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	AltConf	Trace
6	F	4	Total C N O 56 32 4 20	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

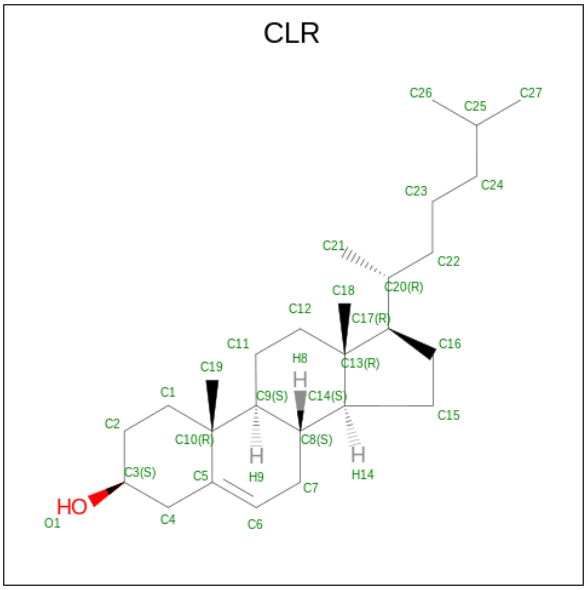
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Ca 1 1	0
7	D	1	Total Ca 1 1	0

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



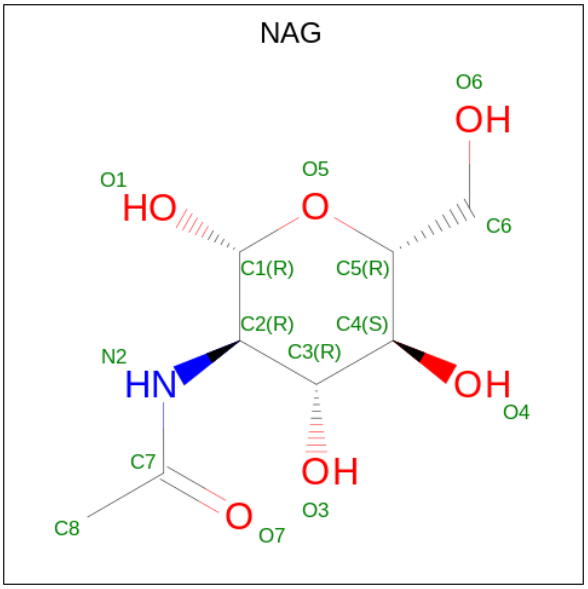
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



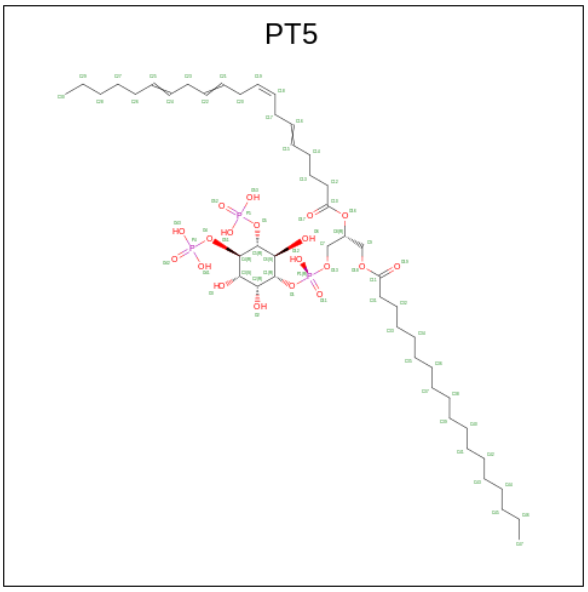
Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	
9	A	1	Total	C	O	0
			28	27	1	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



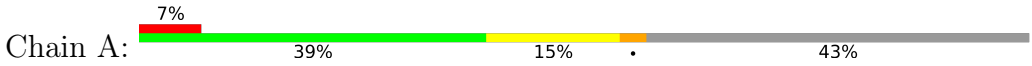
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			63	41	19	3	

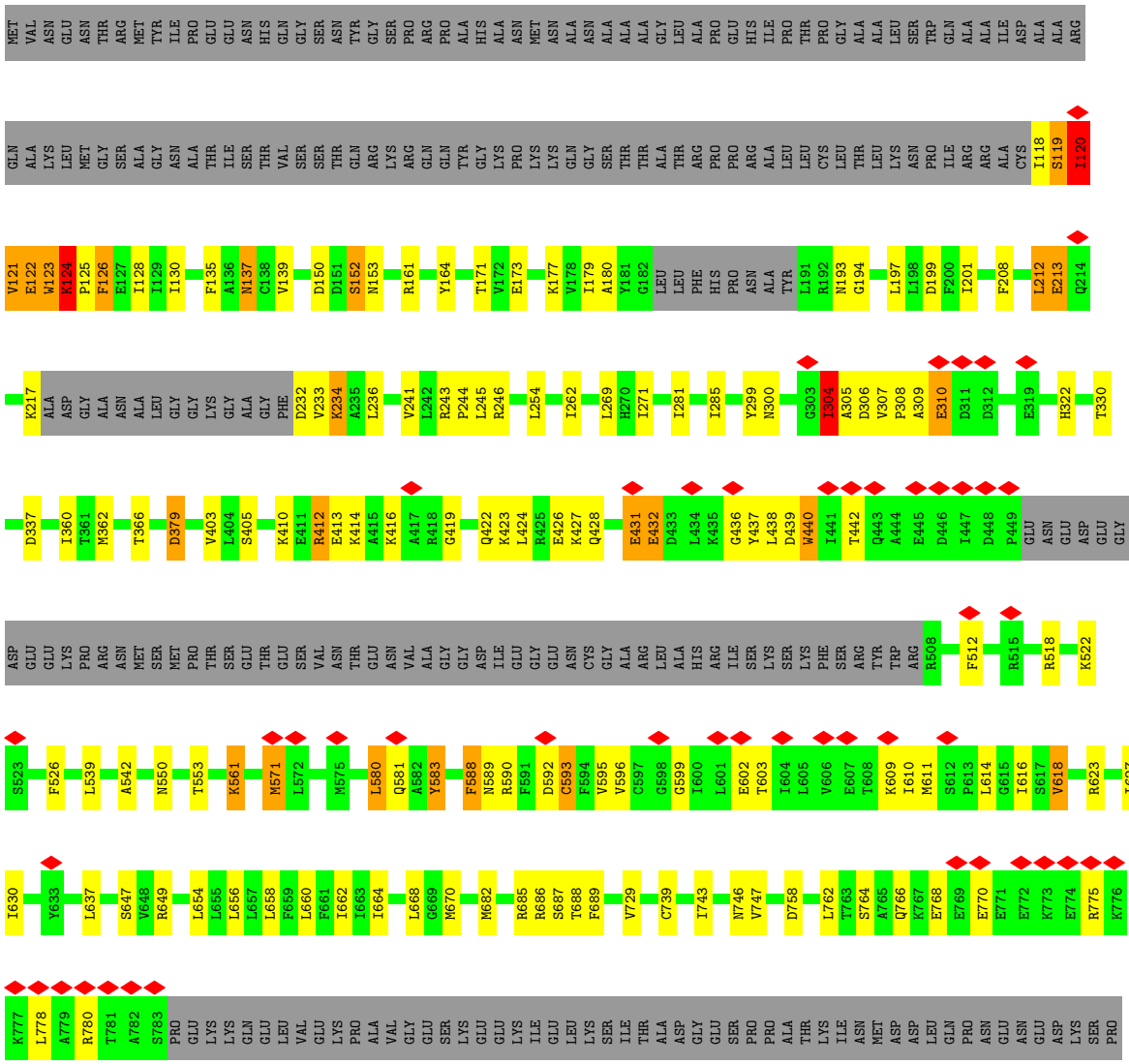
3 Residue-property plots (i)

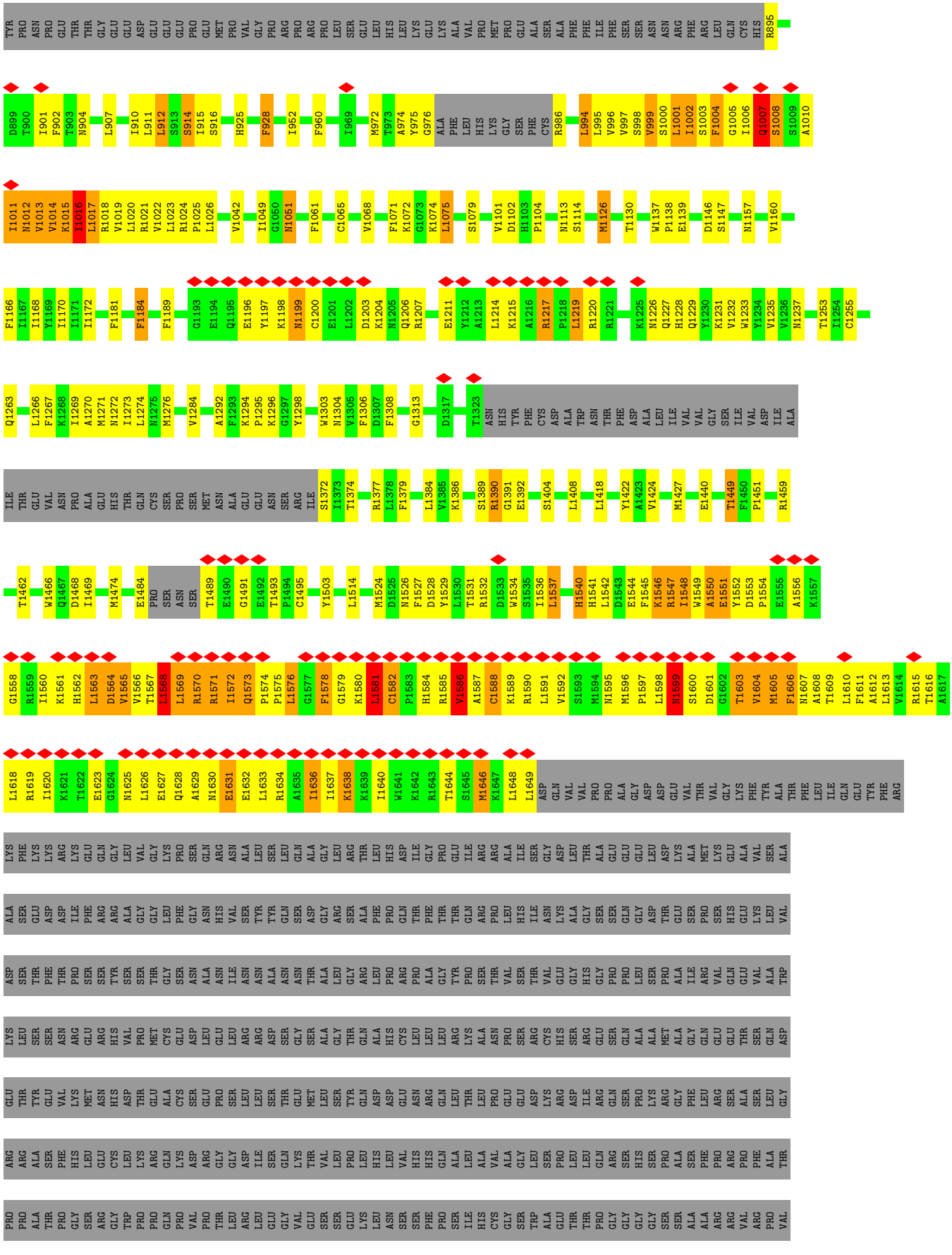
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

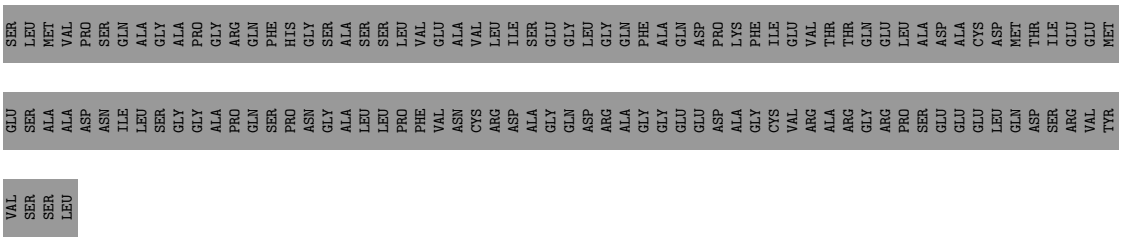
• Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1C

Chain A:



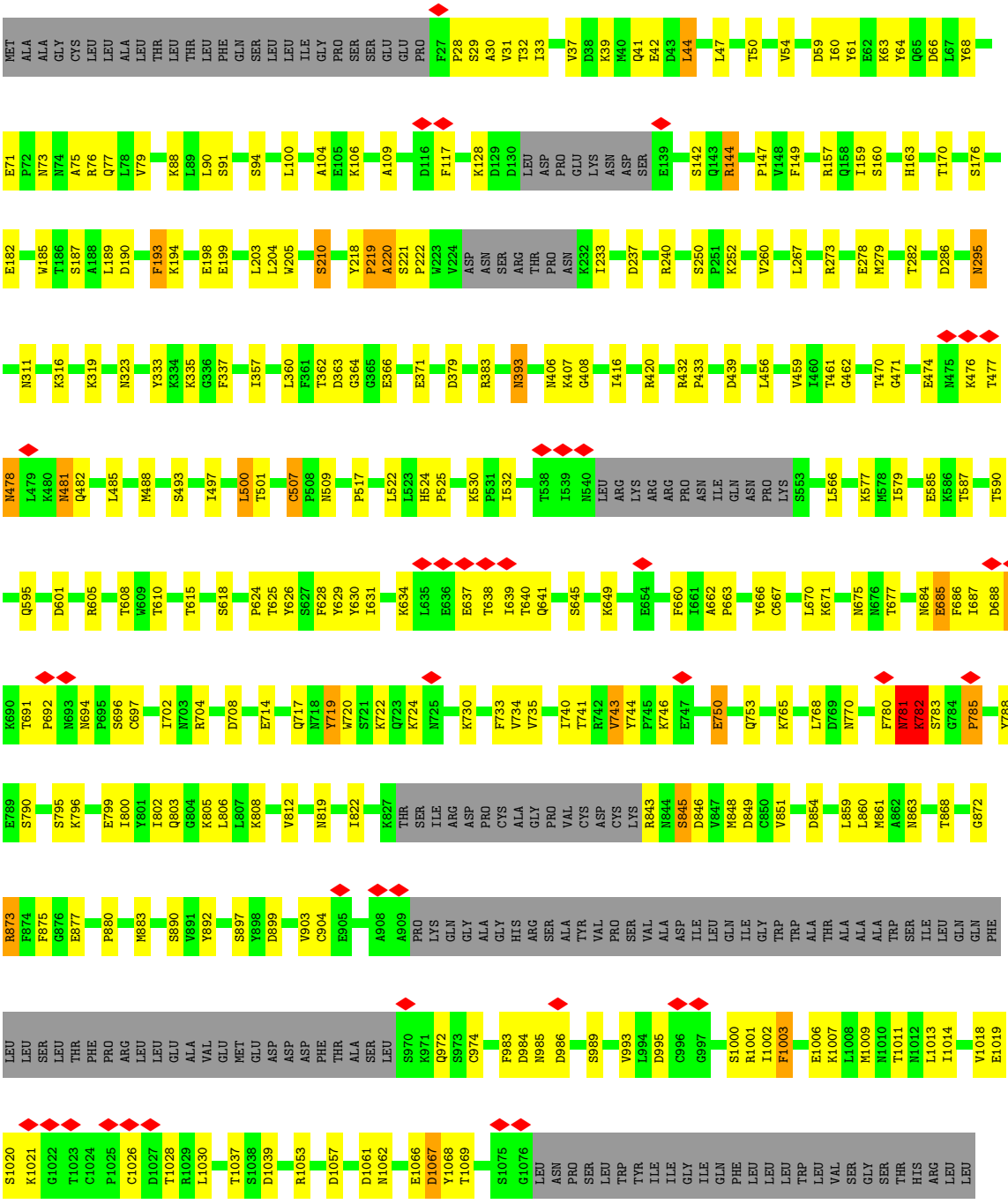






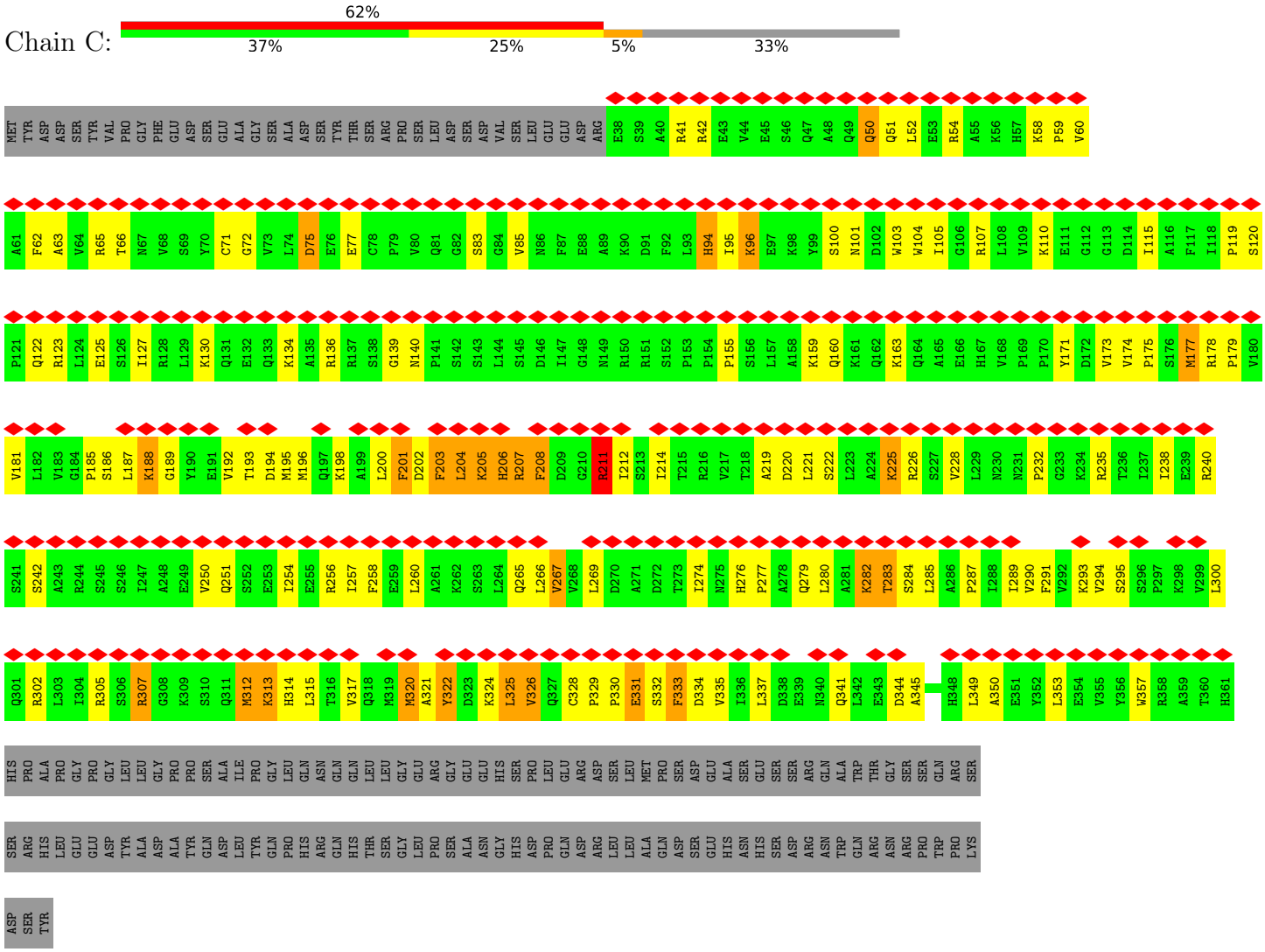
• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:



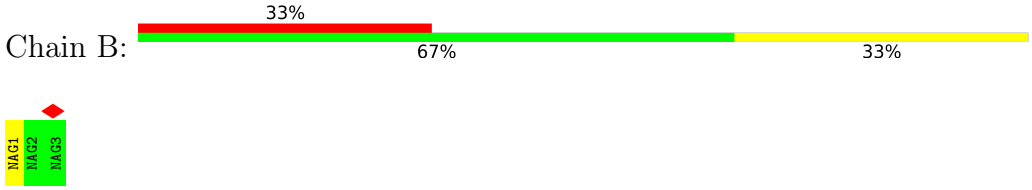
• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:



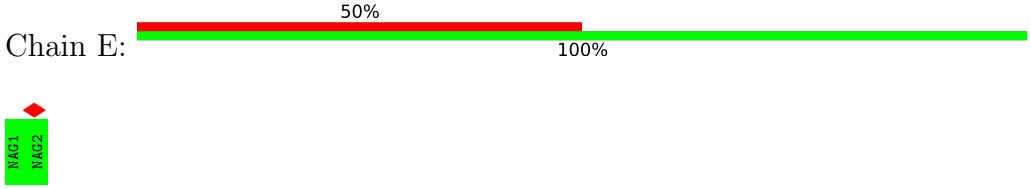
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:



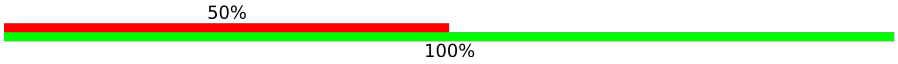
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



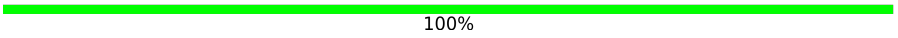
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	217938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.006	Depositor
Minimum map value	-1.886	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CA, PT5, NAG, CLR

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	0.34	0/10402	0.53	0/14093
2	D	0.32	0/7728	0.50	0/10477
3	C	0.28	0/2624	0.55	0/3544
All	All	0.32	0/20754	0.52	0/28114

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

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	10172	0	10395	329	0
2	D	7570	0	7369	171	0
3	C	2575	0	2619	118	0
4	B	42	0	37	0	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	0	0
6	F	56	0	49	3	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	40	0	54	1	0
9	A	84	0	138	5	0
10	A	14	0	13	0	0
10	D	28	0	26	0	0
11	A	63	0	66	2	0
All	All	20730	0	20841	617	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 (617) 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)
3:C:203:PHE:CZ	3:C:350:ALA:HB2	1.61	1.32
1:A:1560:ILE:HG12	1:A:1603:THR:HA	1.33	1.11
3:C:203:PHE:HZ	3:C:350:ALA:HB2	0.96	1.06
3:C:203:PHE:HZ	3:C:350:ALA:CB	1.67	1.06
2:D:780:PHE:HB2	2:D:873:ARG:HG2	1.43	1.00
1:A:1561:LYS:HE3	1:A:1563:LEU:HD23	1.54	0.89
1:A:1585:ARG:HD3	1:A:1587:ALA:HB3	1.55	0.89
1:A:1588:CYS:HA	1:A:1591:LEU:HG	1.60	0.84
3:C:204:LEU:HD23	3:C:349:LEU:HD21	1.60	0.84
3:C:276:HIS:CE1	3:C:328:CYS:HB3	2.12	0.84
1:A:1003:SER:HB2	1:A:1017:LEU:HD11	1.63	0.81
1:A:122:GLU:O	1:A:123:TRP:HB2	1.83	0.78
1:A:1197:TYR:O	1:A:1198:LYS:HG2	1.84	0.78
3:C:211:ARG:NH2	3:C:353:LEU:HD13	1.99	0.78
3:C:205:LYS:HA	3:C:212:ILE:HG21	1.66	0.77
1:A:1563:LEU:HA	1:A:1566:VAL:HG22	1.65	0.77
2:D:780:PHE:CB	2:D:873:ARG:HG2	2.14	0.77
1:A:1266:LEU:HD12	1:A:1269:ILE:HD11	1.65	0.76
2:D:649:LYS:HD3	2:D:684:ASN:HD21	1.51	0.76
2:D:357:ILE:HG22	2:D:383:ARG:HB2	1.68	0.75
3:C:289:ILE:HG22	3:C:333:PHE:HB3	1.68	0.75
1:A:299:TYR:HB3	1:A:304:ILE:HG21	1.67	0.75
3:C:203:PHE:O	3:C:207:ARG:HB3	1.87	0.74
2:D:780:PHE:O	2:D:781:ASN:HB3	1.87	0.73
3:C:290:VAL:HG22	3:C:335:VAL:HB	1.71	0.73
1:A:1560:ILE:CG1	1:A:1603:THR:HA	2.17	0.73
3:C:211:ARG:HG3	3:C:357:TRP:CD1	2.23	0.73
2:D:199:GLU:OE2	2:D:199:GLU:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:GLN:O	3:C:50:GLN:NE2	2.22	0.72
1:A:1253:THR:HG21	1:A:1384:LEU:HD13	1.72	0.72
1:A:1637:ILE:HG23	1:A:1638:LYS:HD2	1.72	0.72
2:D:860:LEU:HD12	2:D:1013:LEU:HD11	1.71	0.71
2:D:295:ASN:O	2:D:295:ASN:ND2	2.20	0.71
1:A:121:VAL:O	1:A:122:GLU:C	2.29	0.70
1:A:212:LEU:HB3	1:A:233:VAL:HG13	1.72	0.69
1:A:1569:LEU:HD11	1:A:1581:LEU:H	1.57	0.69
2:D:780:PHE:CD1	2:D:873:ARG:HA	2.28	0.69
3:C:203:PHE:CZ	3:C:350:ALA:CB	2.50	0.69
3:C:207:ARG:HG3	3:C:208:PHE:CD1	2.28	0.68
1:A:1597:PRO:HD2	1:A:1599:ASN:HD21	1.59	0.68
1:A:1640:ILE:HG21	1:A:1644:THR:HG23	1.74	0.68
3:C:285:LEU:HD12	3:C:287:PRO:HD3	1.74	0.68
3:C:179:PRO:HB2	3:C:287:PRO:HB3	1.76	0.68
2:D:109:ALA:HA	2:D:470:THR:HG22	1.75	0.68
1:A:1544:GLU:O	1:A:1548:ILE:HG23	1.94	0.67
2:D:159:ILE:HG22	2:D:221:SER:HB2	1.75	0.67
2:D:708:ASP:HB3	2:D:740:ILE:HD11	1.76	0.67
2:D:1001:ARG:HG2	2:D:1001:ARG:HH11	1.60	0.67
1:A:1625:ASN:HA	1:A:1628:GLN:HB2	1.76	0.67
3:C:177:MET:CE	3:C:211:ARG:HD3	2.25	0.67
2:D:41:GLN:HE21	2:D:1009:MET:HB2	1.58	0.67
1:A:123:TRP:CD2	1:A:125:PRO:HD2	2.29	0.66
1:A:1006:ILE:HD12	1:A:1008:SER:H	1.60	0.66
2:D:601:ASP:OD1	2:D:770:ASN:ND2	2.28	0.65
1:A:1604:VAL:HG13	1:A:1608:ALA:HB3	1.77	0.65
1:A:213:GLU:OE1	1:A:233:VAL:HG12	1.97	0.65
3:C:329:PRO:HB2	3:C:331:GLU:HG3	1.77	0.65
1:A:437:TYR:HE2	3:C:294:VAL:HA	1.59	0.65
1:A:118:ILE:N	1:A:121:VAL:HB	2.12	0.65
1:A:179:ILE:O	1:A:179:ILE:HD12	1.96	0.65
1:A:1440:GLU:HG3	1:A:1468:ASP:HB3	1.79	0.64
3:C:312:MET:SD	3:C:312:MET:N	2.71	0.64
1:A:300:ASN:N	1:A:308:PRO:HG3	2.13	0.64
1:A:1569:LEU:HD12	1:A:1578:PHE:HB3	1.81	0.63
1:A:1196:GLU:HG2	1:A:1198:LYS:H	1.62	0.63
2:D:800:ILE:HD12	2:D:802:ILE:HD11	1.81	0.63
1:A:1569:LEU:HA	1:A:1572:ILE:HG12	1.79	0.63
2:D:482:GLN:HE22	2:D:1067:ASP:HB2	1.63	0.63
1:A:1001:LEU:HA	1:A:1004:PHE:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:GLN:HB3	1:A:1576:LEU:HD21	1.80	0.62
2:D:260:VAL:HG23	2:D:295:ASN:HB3	1.81	0.62
1:A:124:LYS:HB2	1:A:125:PRO:HD3	1.80	0.62
1:A:299:TYR:HA	1:A:308:PRO:HD2	1.82	0.62
1:A:254:LEU:HD21	1:A:656:LEU:HD23	1.80	0.62
3:C:283:THR:OG1	3:C:284:SER:N	2.33	0.62
1:A:1561:LYS:C	1:A:1563:LEU:H	2.03	0.62
1:A:412:ARG:NH1	1:A:758:ASP:OD1	2.28	0.62
3:C:208:PHE:CE1	3:C:353:LEU:HD11	2.35	0.61
1:A:1574:PRO:HD3	1:A:1579:GLY:HA2	1.82	0.61
2:D:237:ASP:OD2	2:D:420:ARG:NH1	2.34	0.61
3:C:177:MET:HE1	3:C:211:ARG:HD3	1.82	0.61
1:A:602:GLU:HG3	1:A:616:ILE:HG12	1.81	0.61
2:D:477:THR:HG23	2:D:481:ASN:HD22	1.64	0.61
3:C:181:VAL:HG22	3:C:269:LEU:HD11	1.83	0.61
2:D:90:LEU:HD12	2:D:615:THR:HG21	1.82	0.61
1:A:1568:LEU:HD12	1:A:1570:ARG:NH2	2.15	0.61
1:A:1578:PHE:HD2	1:A:1591:LEU:HD11	1.65	0.61
1:A:1569:LEU:CD1	1:A:1578:PHE:HB3	2.31	0.60
1:A:1615:ARG:HD3	1:A:1620:ILE:HA	1.83	0.60
1:A:1489:THR:HG23	1:A:1491:GLY:H	1.67	0.60
1:A:1598:LEU:HD22	1:A:1648:LEU:HB2	1.82	0.60
1:A:118:ILE:CA	1:A:121:VAL:HB	2.31	0.60
2:D:750:GLU:OE2	2:D:750:GLU:N	2.33	0.60
3:C:206:HIS:N	3:C:206:HIS:CD2	2.70	0.60
3:C:211:ARG:HD2	3:C:211:ARG:O	2.02	0.60
1:A:1071:PHE:HB3	1:A:1075:LEU:HD11	1.83	0.60
1:A:1599:ASN:HB3	1:A:1605:MET:HG2	1.83	0.60
1:A:1549:TRP:CH2	1:A:1606:PHE:HA	2.37	0.59
2:D:753:GLN:OE1	2:D:753:GLN:N	2.36	0.59
1:A:1014:VAL:HA	1:A:1017:LEU:HD22	1.84	0.59
2:D:407:LYS:NZ	2:D:1062:ASN:OD1	2.34	0.59
1:A:1021:ARG:O	1:A:1023:LEU:N	2.35	0.59
1:A:1633:LEU:HD21	1:A:1640:ILE:HD11	1.85	0.59
3:C:206:HIS:CD2	3:C:206:HIS:H	2.21	0.59
3:C:186:SER:OG	3:C:187:LEU:N	2.36	0.59
1:A:1627:GLU:HA	1:A:1630:ASN:HB2	1.85	0.59
1:A:1560:ILE:HG12	1:A:1603:THR:CA	2.23	0.59
1:A:686:ARG:NH2	1:A:1146:ASP:OD1	2.35	0.58
1:A:1220:ARG:HH12	1:A:1556:ALA:HB2	1.68	0.58
3:C:256:ARG:HA	3:C:260:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1561:LYS:H	1:A:1564:ASP:CG	2.07	0.58
1:A:1626:LEU:HD12	1:A:1627:GLU:H	1.67	0.58
1:A:1231:LYS:O	1:A:1235:VAL:HG23	2.04	0.58
1:A:1541:HIS:HB3	1:A:1576:LEU:HB3	1.85	0.58
3:C:322:TYR:O	3:C:326:VAL:HG23	2.03	0.58
1:A:1011:ILE:O	1:A:1012:ASN:C	2.39	0.58
1:A:1596:MET:SD	1:A:1601:ASP:N	2.77	0.58
1:A:1012:ASN:O	1:A:1014:VAL:N	2.37	0.58
1:A:118:ILE:C	1:A:120:ILE:H	2.07	0.58
1:A:1585:ARG:O	1:A:1588:CYS:N	2.37	0.58
1:A:1269:ILE:O	1:A:1273:ILE:HG13	2.03	0.58
3:C:75:ASP:OD1	3:C:123:ARG:NH2	2.37	0.58
1:A:1550:ALA:O	1:A:1551:GLU:C	2.42	0.58
2:D:667:CYS:HA	2:D:697:CYS:HB2	1.85	0.58
1:A:1549:TRP:O	1:A:1550:ALA:C	2.40	0.57
1:A:1562:HIS:O	1:A:1566:VAL:HG13	2.03	0.57
1:A:1295:PRO:HD2	1:A:1296:LYS:H	1.68	0.57
1:A:599:GLY:O	1:A:603:THR:HG23	2.05	0.57
2:D:1011:THR:HG22	2:D:1013:LEU:H	1.70	0.57
1:A:1200:CYS:HB3	1:A:1636:ILE:HD12	1.86	0.57
1:A:1585:ARG:O	1:A:1586:VAL:C	2.40	0.57
3:C:127:ILE:HG23	3:C:130:LYS:HD3	1.85	0.57
3:C:202:ASP:HA	3:C:206:HIS:CD2	2.40	0.57
1:A:1569:LEU:HD23	1:A:1570:ARG:CZ	2.36	0.56
3:C:212:ILE:N	3:C:265:GLN:HE21	2.03	0.56
3:C:211:ARG:HH21	3:C:353:LEU:HD13	1.69	0.56
2:D:29:SER:OG	2:D:30:ALA:N	2.37	0.56
3:C:174:VAL:HG11	3:C:178:ARG:HH11	1.70	0.56
1:A:1021:ARG:C	1:A:1023:LEU:H	2.09	0.56
1:A:1596:MET:SD	1:A:1601:ASP:HA	2.45	0.56
2:D:780:PHE:HB3	2:D:873:ARG:N	2.21	0.56
2:D:198:GLU:OE1	2:D:198:GLU:N	2.39	0.56
1:A:581:GLN:OE1	1:A:581:GLN:N	2.39	0.56
6:F:3:NAG:H83	6:F:3:NAG:H3	1.88	0.56
1:A:1126:MET:O	1:A:1130:THR:HG23	2.06	0.55
3:C:195:MET:HA	3:C:198:LYS:HG3	1.88	0.55
1:A:1313:GLY:HA3	1:A:1379:PHE:HD2	1.71	0.55
2:D:193:PHE:HB3	2:D:218:TYR:HD2	1.72	0.55
3:C:203:PHE:CE2	3:C:350:ALA:HB2	2.33	0.55
1:A:119:SER:HB3	1:A:179:ILE:O	2.07	0.55
1:A:1013:VAL:O	1:A:1014:VAL:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302:ARG:HA	3:C:305:ARG:HG2	1.89	0.55
1:A:241:VAL:HG21	1:A:668:LEU:HB2	1.89	0.55
1:A:1564:ASP:HA	1:A:1567:THR:HG22	1.88	0.55
2:D:149:PHE:CZ	2:D:222:PRO:HD3	2.42	0.55
1:A:121:VAL:O	1:A:123:TRP:N	2.40	0.55
1:A:1006:ILE:HG13	1:A:1007:GLN:N	2.22	0.55
1:A:901:ILE:HG13	1:A:902:PHE:N	2.23	0.54
1:A:1010:ALA:O	1:A:1012:ASN:N	2.40	0.54
1:A:125:PRO:HA	1:A:128:ILE:HG12	1.89	0.54
6:F:4:NAG:H3	6:F:4:NAG:H83	1.88	0.54
1:A:1018:ARG:O	1:A:1021:ARG:HG3	2.08	0.54
3:C:125:GLU:O	3:C:160:GLN:NE2	2.41	0.54
2:D:218:TYR:HB3	2:D:219:PRO:HD3	1.88	0.54
1:A:300:ASN:H	1:A:308:PRO:HG3	1.73	0.54
2:D:625:THR:HG22	2:D:626:TYR:H	1.71	0.54
2:D:638:THR:HG22	2:D:692:PRO:HG2	1.89	0.54
2:D:1001:ARG:HG2	2:D:1001:ARG:NH1	2.22	0.54
1:A:1569:LEU:HD11	1:A:1581:LEU:HG	1.90	0.54
1:A:1551:GLU:HG3	1:A:1552:TYR:CZ	2.42	0.54
1:A:1228:HIS:HA	1:A:1231:LYS:HE3	1.88	0.54
1:A:1605:MET:O	1:A:1607:ASN:N	2.40	0.54
2:D:471:GLY:HA3	2:D:476:LYS:HE2	1.89	0.54
2:D:904:CYS:N	2:D:972:GLN:O	2.36	0.54
3:C:95:ILE:HD13	3:C:104:TRP:HB3	1.89	0.54
1:A:1199:ASN:O	1:A:1199:ASN:ND2	2.29	0.53
1:A:137:ASN:OD1	1:A:243:ARG:NH1	2.40	0.53
1:A:1561:LYS:HG3	1:A:1563:LEU:HB2	1.89	0.53
3:C:201:PHE:O	3:C:202:ASP:C	2.46	0.53
1:A:1598:LEU:HD13	1:A:1648:LEU:HB3	1.91	0.53
3:C:225:LYS:NZ	3:C:279:GLN:O	2.41	0.53
3:C:276:HIS:HE1	3:C:328:CYS:HB3	1.71	0.53
2:D:780:PHE:HB3	2:D:872:GLY:C	2.28	0.53
2:D:1003:PHE:HB3	2:D:1018:VAL:HG22	1.89	0.53
3:C:192:VAL:HG23	3:C:307:ARG:HE	1.73	0.53
1:A:1137:TRP:CD1	1:A:1138:PRO:HD3	2.44	0.53
2:D:641:GLN:O	2:D:645:SER:OG	2.26	0.53
1:A:1269:ILE:HD12	1:A:1270:ALA:N	2.24	0.53
1:A:999:VAL:O	1:A:1000:SER:C	2.47	0.53
1:A:1203:ASP:HB3	1:A:1619:ARG:HH21	1.74	0.53
1:A:1598:LEU:HB2	1:A:1648:LEU:H	1.74	0.53
2:D:720:TRP:HE3	2:D:744:TYR:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:843:ARG:N	2:D:845:SER:HG	2.07	0.53
1:A:1569:LEU:HD23	1:A:1570:ARG:NH1	2.24	0.52
2:D:1039:ASP:N	2:D:1039:ASP:OD1	2.42	0.52
3:C:205:LYS:HB3	3:C:206:HIS:HD2	1.73	0.52
2:D:240:ARG:NH2	2:D:278:GLU:O	2.42	0.52
1:A:685:ARG:O	1:A:688:THR:HG23	2.10	0.52
1:A:424:LEU:HG	1:A:762:LEU:HD11	1.92	0.52
2:D:205:TRP:HE1	2:D:456:LEU:HD22	1.74	0.52
1:A:300:ASN:O	1:A:304:ILE:HG12	2.10	0.52
2:D:100:LEU:HB3	2:D:488:MET:CE	2.40	0.52
3:C:257:ILE:HG22	3:C:258:PHE:H	1.75	0.51
1:A:193:ASN:OD1	1:A:194:GLY:N	2.43	0.51
1:A:304:ILE:C	1:A:306:ASP:H	2.12	0.51
1:A:1272:ASN:O	1:A:1276:MET:HG3	2.11	0.51
1:A:1203:ASP:O	1:A:1206:GLN:N	2.38	0.51
1:A:1584:HIS:O	1:A:1585:ARG:C	2.47	0.51
2:D:459:VAL:HG12	2:D:493:SER:HA	1.92	0.51
1:A:1157:ASN:HD22	2:D:393:ASN:HD22	1.59	0.51
1:A:729:VAL:HA	9:A:2304:CLR:H151	1.92	0.51
1:A:1233:TRP:O	1:A:1237:ASN:HB2	2.10	0.51
1:A:1552:TYR:O	1:A:1553:ASP:HB2	2.11	0.51
2:D:273:ARG:HD2	2:D:323:ASN:HA	1.93	0.51
3:C:293:LYS:HG3	3:C:295:SER:H	1.75	0.51
3:C:313:LYS:HG3	3:C:314:HIS:CD2	2.45	0.51
1:A:1528:ASP:OD1	1:A:1529:TYR:N	2.44	0.51
1:A:1549:TRP:CZ3	1:A:1606:PHE:HD1	2.28	0.51
1:A:1551:GLU:HG2	1:A:1552:TYR:H	1.75	0.51
1:A:1568:LEU:HA	1:A:1571:ARG:HH22	1.76	0.51
2:D:671:LYS:HB2	2:D:671:LYS:NZ	2.26	0.51
1:A:1199:ASN:HD22	1:A:1199:ASN:C	2.10	0.51
1:A:1561:LYS:C	1:A:1563:LEU:N	2.63	0.51
2:D:993:VAL:HG22	2:D:1002:ILE:HG22	1.92	0.51
2:D:104:ALA:HB2	2:D:189:LEU:HD21	1.92	0.51
1:A:123:TRP:CG	1:A:125:PRO:HD2	2.45	0.51
1:A:1390:ARG:HD2	1:A:1391:GLY:N	2.26	0.51
2:D:629:TYR:HE2	2:D:805:LYS:HZ2	1.59	0.50
1:A:1631:GLU:HA	1:A:1634:ARG:HG2	1.93	0.50
2:D:163:HIS:O	2:D:220:ALA:HB2	2.12	0.50
2:D:802:ILE:HG22	2:D:803:GLN:OE1	2.11	0.50
3:C:202:ASP:O	3:C:203:PHE:C	2.49	0.50
1:A:199:ASP:OD2	1:A:246:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:PHE:O	3:C:204:LEU:HG	2.12	0.50
1:A:907:LEU:HA	1:A:910:ILE:HD12	1.93	0.50
1:A:1303:TRP:HE1	11:A:2307:PT5:H15	1.75	0.50
1:A:1572:ILE:HG13	1:A:1578:PHE:H	1.76	0.50
3:C:280:LEU:HD21	3:C:289:ILE:HD11	1.93	0.50
1:A:432:GLU:O	1:A:436:GLY:N	2.43	0.50
1:A:911:LEU:O	1:A:915:ILE:HG13	2.10	0.50
1:A:1010:ALA:O	1:A:1011:ILE:C	2.49	0.50
1:A:1568:LEU:HA	1:A:1571:ARG:NH2	2.27	0.50
1:A:1569:LEU:HD11	1:A:1581:LEU:N	2.27	0.50
1:A:410:LYS:O	1:A:414:LYS:HG2	2.11	0.50
1:A:998:SER:O	1:A:999:VAL:C	2.50	0.50
1:A:1166:PHE:O	1:A:1170:ILE:HD12	2.11	0.50
1:A:1560:ILE:HD12	1:A:1565:VAL:HG21	1.93	0.50
1:A:1006:ILE:O	1:A:1008:SER:N	2.45	0.50
3:C:225:LYS:HE3	3:C:282:LYS:HE3	1.94	0.50
1:A:743:ILE:O	1:A:747:VAL:HB	2.12	0.50
3:C:334:ASP:CG	3:C:335:VAL:HG23	2.32	0.50
1:A:119:SER:HB3	1:A:180:ALA:HA	1.94	0.50
1:A:729:VAL:HG23	9:A:2304:CLR:H151	1.93	0.50
1:A:1211:GLU:O	1:A:1215:LYS:HG2	2.12	0.50
1:A:1595:ASN:O	1:A:1597:PRO:HD3	2.12	0.50
2:D:750:GLU:H	2:D:750:GLU:CD	2.15	0.50
3:C:203:PHE:O	3:C:204:LEU:C	2.50	0.50
3:C:211:ARG:O	3:C:265:GLN:HA	2.12	0.50
1:A:1294:LYS:HD3	1:A:1295:PRO:HD3	1.93	0.49
3:C:331:GLU:O	3:C:332:SER:C	2.49	0.49
1:A:422:GLN:O	1:A:426:GLU:HG2	2.10	0.49
1:A:1074:LYS:HB3	1:A:1147:SER:HB2	1.94	0.49
1:A:1560:ILE:CD1	1:A:1604:VAL:H	2.25	0.49
1:A:1560:ILE:HD13	1:A:1604:VAL:H	1.77	0.49
2:D:733:PHE:HB3	2:D:743:VAL:HG13	1.95	0.49
2:D:843:ARG:N	2:D:845:SER:OG	2.45	0.49
2:D:1007:LYS:HG2	2:D:1014:ILE:HD13	1.95	0.49
1:A:994:LEU:O	1:A:997:VAL:HG12	2.13	0.49
1:A:1626:LEU:HD12	1:A:1627:GLU:N	2.26	0.49
2:D:781:ASN:O	2:D:782:LYS:HB2	2.10	0.49
3:C:328:CYS:HB2	3:C:329:PRO:HD2	1.95	0.49
1:A:1204:LYS:HE2	1:A:1204:LYS:N	2.28	0.49
2:D:28:PRO:HB2	2:D:33:ILE:HG13	1.95	0.49
1:A:299:TYR:HA	1:A:308:PRO:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:LYS:NZ	3:C:274:ILE:O	2.30	0.49
1:A:197:LEU:O	1:A:201:ILE:HG23	2.13	0.49
1:A:1104:PRO:HB2	2:D:233:ILE:HG21	1.94	0.49
2:D:182:GLU:OE1	2:D:210:SER:OG	2.27	0.49
1:A:1630:ASN:O	1:A:1633:LEU:HD23	2.13	0.49
2:D:694:ASN:O	2:D:696:SER:N	2.43	0.49
3:C:139:GLY:HA3	3:C:155:PRO:HD2	1.95	0.49
1:A:1199:ASN:ND2	1:A:1199:ASN:C	2.64	0.49
1:A:1541:HIS:CD2	1:A:1576:LEU:HD22	2.48	0.49
3:C:60:VAL:HA	3:C:96:LYS:HD2	1.94	0.49
1:A:1217:ARG:NH2	1:A:1607:ASN:HD21	2.11	0.49
3:C:240:ARG:NE	3:C:242:SER:OG	2.46	0.49
1:A:439:ASP:HB2	3:C:341:GLN:OE1	2.13	0.48
1:A:1418:LEU:HD22	1:A:1514:LEU:HD12	1.95	0.48
3:C:71:CYS:SG	3:C:72:GLY:N	2.85	0.48
1:A:542:ALA:HB2	1:A:1061:PHE:HZ	1.79	0.48
3:C:221:LEU:HD21	3:C:285:LEU:HD22	1.95	0.48
2:D:685:GLU:OE1	2:D:689:ARG:NH1	2.45	0.48
3:C:226:ARG:HH11	3:C:254:ILE:HD11	1.78	0.48
1:A:1545:PHE:O	1:A:1546:LYS:C	2.51	0.48
1:A:1567:THR:O	1:A:1570:ARG:HB2	2.14	0.48
1:A:246:ARG:HE	1:A:246:ARG:HB3	1.41	0.48
1:A:1006:ILE:O	1:A:1007:GLN:C	2.51	0.48
1:A:1574:PRO:C	1:A:1576:LEU:H	2.17	0.48
3:C:205:LYS:HB2	3:C:214:ILE:HD11	1.96	0.48
1:A:588:PHE:HZ	1:A:623:ARG:HA	1.78	0.48
2:D:507:CYS:SG	2:D:509:ASN:N	2.81	0.48
3:C:173:VAL:O	3:C:284:SER:OG	2.31	0.48
2:D:76:ARG:HH21	2:D:610:THR:HG23	1.79	0.48
3:C:317:VAL:HA	3:C:320:MET:SD	2.53	0.48
1:A:925:HIS:CE1	1:A:1484:GLU:H	2.32	0.47
1:A:1560:ILE:HD13	1:A:1604:VAL:HB	1.96	0.47
11:A:2307:PT5:H56	11:A:2307:PT5:H34	1.95	0.47
2:D:63:LYS:HG3	2:D:64:TYR:CD1	2.49	0.47
2:D:851:VAL:HG23	2:D:861:MET:O	2.13	0.47
1:A:123:TRP:CE2	1:A:125:PRO:HD2	2.49	0.47
1:A:152:SER:OG	1:A:153:ASN:N	2.47	0.47
3:C:295:SER:O	3:C:322:TYR:OH	2.33	0.47
1:A:1374:THR:HA	1:A:1377:ARG:HD3	1.96	0.47
1:A:1012:ASN:O	1:A:1013:VAL:C	2.53	0.47
2:D:524:HIS:CD2	2:D:525:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:TRP:HD1	3:C:120:SER:HB2	1.79	0.47
1:A:1013:VAL:HA	1:A:1016:ILE:HG22	1.97	0.47
1:A:1018:ARG:C	1:A:1020:LEU:H	2.18	0.47
1:A:304:ILE:C	1:A:306:ASP:N	2.68	0.47
1:A:1229:GLN:HE22	1:A:1294:LYS:HE3	1.80	0.47
1:A:1563:LEU:HA	1:A:1566:VAL:CG2	2.38	0.47
1:A:1589:LYS:HA	1:A:1592:VAL:HG23	1.97	0.47
2:D:637:GLU:HG3	2:D:639:ILE:HG13	1.95	0.47
1:A:119:SER:OG	1:A:179:ILE:HD12	2.15	0.47
1:A:379:ASP:N	1:A:379:ASP:OD1	2.48	0.47
1:A:1168:ILE:HG23	1:A:1172:ILE:HD12	1.96	0.47
2:D:90:LEU:O	2:D:94:SER:OG	2.32	0.47
2:D:193:PHE:HB3	2:D:218:TYR:CD2	2.48	0.47
1:A:118:ILE:HA	1:A:121:VAL:HB	1.95	0.47
1:A:762:LEU:O	1:A:766:GLN:HG2	2.14	0.47
1:A:1011:ILE:O	1:A:1013:VAL:N	2.48	0.47
2:D:157:ARG:NH2	2:D:222:PRO:O	2.47	0.47
2:D:875:PHE:HB3	2:D:883:MET:SD	2.55	0.47
2:D:734:VAL:HG22	2:D:812:VAL:HG12	1.97	0.47
3:C:294:VAL:HG11	3:C:300:LEU:HD13	1.95	0.47
1:A:1630:ASN:O	1:A:1634:ARG:HB3	2.14	0.46
2:D:904:CYS:SG	2:D:974:CYS:N	2.88	0.46
3:C:212:ILE:C	3:C:265:GLN:NE2	2.69	0.46
1:A:1296:LYS:HA	1:A:1296:LYS:HD3	1.65	0.46
2:D:765:LYS:HA	2:D:768:LEU:HD12	1.95	0.46
2:D:44:LEU:HA	2:D:47:LEU:HB3	1.98	0.46
1:A:119:SER:HB3	1:A:180:ALA:HB2	1.98	0.46
3:C:219:ALA:HB1	3:C:250:VAL:HG23	1.96	0.46
1:A:124:LYS:CB	1:A:125:PRO:HD3	2.45	0.46
1:A:1563:LEU:CA	1:A:1566:VAL:HG22	2.40	0.46
1:A:1574:PRO:HA	1:A:1578:PHE:C	2.36	0.46
2:D:279:MET:O	2:D:282:THR:OG1	2.28	0.46
1:A:366:THR:HG21	1:A:1459:ARG:HG3	1.97	0.46
1:A:1214:LEU:HG	1:A:1215:LYS:HD3	1.97	0.46
3:C:276:HIS:CE1	3:C:328:CYS:CB	2.94	0.46
1:A:309:ALA:O	1:A:310:GLU:HB2	2.15	0.46
1:A:571:MET:HE3	1:A:592:ASP:OD2	2.15	0.46
9:A:2304:CLR:H221	9:A:2304:CLR:H162	1.30	0.46
2:D:485:LEU:HD22	6:F:1:NAG:H82	1.97	0.46
1:A:1000:SER:O	1:A:1003:SER:HB3	2.15	0.46
3:C:159:LYS:NZ	3:C:160:GLN:OE1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:477:THR:HG22	2:D:478:ASN:N	2.30	0.46
2:D:688:ASP:OD1	2:D:689:ARG:N	2.49	0.46
2:D:649:LYS:HD3	2:D:684:ASN:ND2	2.26	0.45
1:A:118:ILE:HB	1:A:119:SER:H	1.52	0.45
1:A:658:LEU:O	1:A:662:ILE:HG13	2.16	0.45
1:A:1113:ASN:OD1	1:A:1114:SER:N	2.44	0.45
1:A:1585:ARG:NH1	1:A:1586:VAL:HG13	2.32	0.45
2:D:311:ASN:OD1	2:D:311:ASN:N	2.50	0.45
1:A:1298:TYR:CE1	1:A:1304:ASN:HB3	2.51	0.45
1:A:1596:MET:SD	1:A:1601:ASP:CA	3.04	0.45
1:A:1604:VAL:HG11	1:A:1609:THR:HG23	1.98	0.45
1:A:1628:GLN:N	1:A:1628:GLN:OE1	2.47	0.45
1:A:271:ILE:HD11	1:A:403:VAL:HG21	1.98	0.45
1:A:440:TRP:CD1	3:C:196:MET:HG3	2.51	0.45
1:A:522:LYS:HE2	1:A:522:LYS:HB3	1.70	0.45
1:A:1021:ARG:C	1:A:1023:LEU:N	2.70	0.45
1:A:1267:PHE:O	1:A:1271:MET:HG2	2.17	0.45
1:A:1449:THR:HG22	1:A:1451:PRO:HD2	1.98	0.45
1:A:1547:ARG:O	1:A:1550:ALA:N	2.50	0.45
2:D:730:LYS:HD2	2:D:790:SER:O	2.17	0.45
1:A:299:TYR:HD1	1:A:306:ASP:O	1.99	0.45
1:A:437:TYR:CE2	3:C:294:VAL:HA	2.47	0.45
1:A:1574:PRO:O	1:A:1576:LEU:N	2.50	0.45
2:D:634:LYS:HG2	2:D:634:LYS:O	2.17	0.45
2:D:1061:ASP:OD1	2:D:1061:ASP:N	2.49	0.45
3:C:63:ALA:HA	3:C:94:HIS:HA	1.98	0.45
1:A:118:ILE:C	1:A:120:ILE:N	2.69	0.45
1:A:1569:LEU:HA	1:A:1572:ILE:CG1	2.45	0.45
2:D:42:GLU:N	2:D:42:GLU:OE1	2.50	0.45
2:D:75:ALA:O	2:D:79:VAL:HG23	2.17	0.45
2:D:474:GLU:OE1	2:D:474:GLU:N	2.49	0.45
2:D:477:THR:HG22	2:D:478:ASN:H	1.81	0.45
2:D:781:ASN:CG	2:D:782:LYS:N	2.70	0.45
3:C:205:LYS:C	3:C:207:ARG:H	2.20	0.45
3:C:222:SER:HA	3:C:279:GLN:OE1	2.16	0.45
1:A:670:MET:HA	1:A:689:PHE:HB3	1.98	0.45
1:A:1564:ASP:OD1	1:A:1564:ASP:N	2.49	0.45
1:A:1570:ARG:O	1:A:1580:LYS:HD2	2.17	0.45
1:A:1578:PHE:CE1	1:A:1581:LEU:HD21	2.51	0.45
2:D:117:PHE:CD1	2:D:117:PHE:N	2.84	0.45
1:A:1189:PHE:HB3	1:A:1524:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1550:ALA:O	1:A:1553:ASP:N	2.49	0.45
1:A:1598:LEU:HD23	1:A:1646:MET:C	2.37	0.45
3:C:66:THR:HA	3:C:171:TYR:CD1	2.52	0.45
1:A:1023:LEU:HA	1:A:1026:LEU:HD12	1.99	0.45
1:A:1587:ALA:O	1:A:1590:ARG:HB2	2.16	0.45
2:D:722:LYS:HA	2:D:722:LYS:HD3	1.84	0.45
2:D:890:SER:OG	2:D:890:SER:O	2.34	0.45
2:D:1057:ASP:OD1	2:D:1057:ASP:N	2.42	0.45
2:D:319:LYS:HB3	2:D:319:LYS:HE2	1.77	0.44
2:D:585:GLU:HB3	2:D:608:THR:HG23	1.99	0.44
2:D:785:PRO:HB2	2:D:790:SER:OG	2.17	0.44
3:C:52:LEU:HB3	3:C:115:ILE:HD13	1.99	0.44
3:C:189:GLY:H	3:C:194:ASP:HB2	1.82	0.44
1:A:1313:GLY:HA3	1:A:1379:PHE:CD2	2.51	0.44
1:A:1542:LEU:O	1:A:1545:PHE:HB3	2.16	0.44
1:A:1574:PRO:HA	1:A:1578:PHE:CA	2.47	0.44
2:D:88:LYS:HE3	2:D:88:LYS:HB3	1.79	0.44
2:D:605:ARG:HD3	2:D:624:PRO:HB3	1.99	0.44
1:A:281:ILE:O	1:A:285:ILE:HG13	2.17	0.44
1:A:997:VAL:O	1:A:1001:LEU:HD22	2.17	0.44
2:D:482:GLN:NE2	2:D:1067:ASP:HB2	2.31	0.44
1:A:1102:ASP:OD1	1:A:1102:ASP:N	2.41	0.44
1:A:1606:PHE:O	1:A:1607:ASN:C	2.55	0.44
2:D:714:GLU:HA	2:D:717:GLN:HG3	1.99	0.44
3:C:51:GLN:HA	3:C:54:ARG:HD3	2.00	0.44
3:C:187:LEU:HD12	3:C:187:LEU:H	1.82	0.44
1:A:362:MET:SD	1:A:1462:THR:HG23	2.57	0.44
1:A:593:CYS:HA	1:A:596:VAL:HG12	2.00	0.44
2:D:59:ASP:OD1	2:D:60:ILE:N	2.50	0.44
2:D:788:TYR:OH	2:D:868:THR:HG22	2.18	0.44
1:A:177:LYS:HE2	1:A:177:LYS:HB3	1.82	0.44
1:A:1547:ARG:O	1:A:1549:TRP:N	2.51	0.44
2:D:806:LEU:HD23	2:D:806:LEU:HA	1.77	0.44
1:A:161:ARG:HA	1:A:164:TYR:HD2	1.83	0.44
3:C:100:SER:OG	3:C:101:ASN:N	2.51	0.44
1:A:1226:ASN:HB3	1:A:1229:GLN:HB2	1.99	0.44
1:A:1607:ASN:O	1:A:1608:ALA:C	2.55	0.44
2:D:204:LEU:HD22	2:D:456:LEU:HD21	2.00	0.44
2:D:497:ILE:HA	2:D:500:LEU:HD12	2.00	0.44
3:C:235:ARG:HB2	3:C:238:ILE:HB	1.99	0.44
3:C:330:PRO:O	3:C:331:GLU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:SER:C	1:A:1005:GLY:H	2.21	0.44
2:D:720:TRP:CH2	2:D:734:VAL:HG23	2.53	0.44
3:C:228:VAL:HG11	3:C:232:PRO:HD3	1.99	0.44
2:D:471:GLY:O	2:D:477:THR:OG1	2.36	0.43
3:C:60:VAL:HG11	3:C:107:ARG:NH2	2.33	0.43
1:A:1424:VAL:HA	1:A:1427:MET:HE3	2.00	0.43
2:D:873:ARG:NH2	2:D:877:GLU:O	2.51	0.43
3:C:62:PHE:HD1	3:C:173:VAL:HG11	1.83	0.43
1:A:994:LEU:HD22	1:A:994:LEU:HA	1.72	0.43
1:A:1303:TRP:CZ2	1:A:1389:SER:HB2	2.53	0.43
1:A:1537:LEU:HA	1:A:1541:HIS:ND1	2.33	0.43
1:A:1556:ALA:O	1:A:1558:GLY:N	2.50	0.43
3:C:329:PRO:HB2	3:C:331:GLU:CG	2.48	0.43
1:A:419:GLY:O	1:A:423:LYS:NZ	2.51	0.43
1:A:654:LEU:HB3	1:A:747:VAL:HG22	2.00	0.43
1:A:1611:PHE:O	1:A:1612:ALA:C	2.53	0.43
1:A:120:ILE:HD13	1:A:120:ILE:HA	1.70	0.43
1:A:637:LEU:HD21	1:A:1051:ASN:HB3	2.00	0.43
1:A:1012:ASN:HA	1:A:1015:LYS:CG	2.48	0.43
1:A:1620:ILE:H	1:A:1620:ILE:HD12	1.84	0.43
2:D:660:PHE:HB2	2:D:741:THR:HB	2.00	0.43
2:D:781:ASN:OD1	2:D:782:LYS:HG2	2.18	0.43
2:D:880:PRO:HG3	2:D:1030:LEU:HA	1.99	0.43
1:A:975:TYR:CG	1:A:976:GLY:N	2.86	0.43
1:A:1596:MET:SD	1:A:1600:SER:C	2.97	0.43
2:D:295:ASN:HD22	2:D:295:ASN:C	2.16	0.43
2:D:637:GLU:O	2:D:640:THR:OG1	2.29	0.43
1:A:1598:LEU:CB	1:A:1648:LEU:H	2.32	0.43
2:D:675:ASN:OD1	2:D:677:THR:N	2.52	0.43
3:C:335:VAL:HG12	3:C:337:LEU:CD2	2.47	0.43
1:A:1581:LEU:HB2	1:A:1582:CYS:H	1.65	0.43
1:A:1606:PHE:O	1:A:1608:ALA:N	2.52	0.43
2:D:1001:ARG:NH2	2:D:1020:SER:O	2.46	0.43
1:A:262:ILE:HG13	1:A:262:ILE:O	2.19	0.43
1:A:561:LYS:HA	1:A:561:LYS:HD3	1.71	0.43
1:A:1013:VAL:CA	1:A:1016:ILE:HG22	2.49	0.43
2:D:128:LYS:NZ	2:D:170:THR:HG22	2.34	0.43
3:C:85:VAL:HG21	3:C:119:PRO:HD3	2.00	0.43
3:C:277:PRO:HB2	3:C:332:SER:HB2	1.99	0.43
1:A:739:CYS:O	1:A:743:ILE:HG13	2.19	0.43
1:A:1049:ILE:HD13	1:A:1181:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:LEU:HG	1:A:1546:LYS:HD2	2.01	0.43
1:A:1534:TRP:HE3	1:A:1540:HIS:CD2	2.36	0.43
2:D:481:ASN:OD1	2:D:481:ASN:N	2.52	0.43
2:D:892:TYR:HE1	2:D:983:PHE:CE1	2.37	0.43
3:C:283:THR:HG23	3:C:285:LEU:HG	2.01	0.43
1:A:1013:VAL:O	1:A:1016:ILE:HG22	2.20	0.42
2:D:106:LYS:HE3	2:D:106:LYS:HB3	1.73	0.42
2:D:819:ASN:HA	2:D:822:ILE:HD12	2.01	0.42
1:A:244:PRO:HG2	1:A:664:ILE:HG12	2.01	0.42
1:A:1198:LYS:HD2	1:A:1637:ILE:HG21	2.01	0.42
1:A:1232:VAL:HG12	1:A:1292:ALA:HB2	2.00	0.42
1:A:1466:TRP:HA	1:A:1469:ILE:HD12	2.01	0.42
1:A:1629:ALA:HA	1:A:1632:GLU:HB2	2.01	0.42
2:D:190:ASP:O	2:D:194:LYS:HB2	2.19	0.42
2:D:577:LYS:HB3	2:D:577:LYS:HE2	1.83	0.42
2:D:595:GLN:HB2	2:D:765:LYS:HE3	2.01	0.42
2:D:1066:GLU:HB3	2:D:1068:TYR:CE2	2.54	0.42
1:A:994:LEU:O	1:A:995:LEU:C	2.56	0.42
1:A:1545:PHE:HA	1:A:1548:ILE:HG12	2.01	0.42
2:D:666:TYR:HD2	2:D:702:ILE:HD13	1.84	0.42
3:C:96:LYS:HD3	3:C:96:LYS:H	1.84	0.42
3:C:321:ALA:O	3:C:325:LEU:HD12	2.19	0.42
1:A:1534:TRP:HE3	1:A:1540:HIS:HD2	1.67	0.42
1:A:1560:ILE:HB	1:A:1564:ASP:OD1	2.19	0.42
1:A:1563:LEU:HD12	1:A:1566:VAL:HG21	2.01	0.42
1:A:1578:PHE:CD2	1:A:1591:LEU:HD11	2.51	0.42
1:A:1613:LEU:HA	1:A:1616:THR:HG22	2.02	0.42
2:D:50:THR:O	2:D:719:TYR:OH	2.25	0.42
3:C:291:PHE:CE2	3:C:326:VAL:HG22	2.53	0.42
1:A:912:LEU:HD12	1:A:912:LEU:HA	1.80	0.42
3:C:334:ASP:OD1	3:C:335:VAL:HG23	2.19	0.42
1:A:627:ILE:O	1:A:630:ILE:HG22	2.20	0.42
2:D:735:VAL:HG22	2:D:741:THR:HG23	2.00	0.42
2:D:780:PHE:HD1	2:D:872:GLY:O	2.02	0.42
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.82	0.42
1:A:412:ARG:HE	1:A:412:ARG:HB2	1.66	0.42
1:A:996:VAL:O	1:A:997:VAL:C	2.54	0.42
2:D:144:ARG:HA	2:D:144:ARG:HD3	1.64	0.42
2:D:501:THR:O	2:D:501:THR:OG1	2.32	0.42
2:D:1067:ASP:O	2:D:1068:TYR:HB2	2.19	0.42
1:A:1404:SER:OG	1:A:1526:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:TYR:O	1:A:1503:TYR:OH	2.26	0.42
1:A:1561:LYS:N	1:A:1564:ASP:OD2	2.40	0.42
2:D:859:LEU:HD12	2:D:859:LEU:HA	1.86	0.42
1:A:1581:LEU:HD13	1:A:1585:ARG:HD2	2.02	0.42
9:A:2303:CLR:H162	9:A:2303:CLR:H221	1.50	0.42
3:C:77:GLU:HB3	3:C:103:TRP:CZ2	2.55	0.42
1:A:119:SER:HB3	1:A:180:ALA:CA	2.50	0.41
1:A:130:ILE:CD1	1:A:173:GLU:HG3	2.50	0.41
1:A:153:ASN:N	1:A:153:ASN:OD1	2.50	0.41
1:A:1024:ARG:O	1:A:1025:PRO:C	2.58	0.41
1:A:1206:GLN:HG3	1:A:1619:ARG:HD2	2.02	0.41
1:A:1227:GLN:O	1:A:1231:LYS:HG3	2.20	0.41
1:A:1597:PRO:HD2	1:A:1599:ASN:ND2	2.32	0.41
3:C:174:VAL:HG12	3:C:284:SER:O	2.20	0.41
3:C:207:ARG:HG3	3:C:208:PHE:CE1	2.55	0.41
3:C:266:LEU:HD12	3:C:267:VAL:N	2.35	0.41
1:A:580:LEU:HD23	1:A:581:GLN:H	1.85	0.41
2:D:407:LYS:H	2:D:407:LYS:HG3	1.59	0.41
2:D:780:PHE:CG	2:D:873:ARG:HA	2.55	0.41
1:A:118:ILE:O	1:A:120:ILE:N	2.46	0.41
1:A:1573:GLN:HG2	1:A:1574:PRO:HD2	2.03	0.41
1:A:1634:ARG:HH12	1:A:1644:THR:HG21	1.86	0.41
2:D:147:PRO:HG2	2:D:149:PHE:CZ	2.55	0.41
2:D:182:GLU:HA	2:D:185:TRP:CD1	2.56	0.41
2:D:295:ASN:ND2	2:D:295:ASN:C	2.72	0.41
2:D:363:ASP:OD1	2:D:364:GLY:N	2.50	0.41
2:D:432:ARG:HB2	2:D:433:PRO:HD3	2.02	0.41
2:D:799:GLU:HG2	2:D:808:LYS:HE2	2.02	0.41
3:C:335:VAL:HG12	3:C:337:LEU:HD22	2.03	0.41
1:A:119:SER:HB3	1:A:180:ALA:CB	2.50	0.41
1:A:1562:HIS:O	1:A:1565:VAL:HG23	2.20	0.41
2:D:37:VAL:HG21	2:D:1006:GLU:HG2	2.02	0.41
2:D:1001:ARG:NH2	2:D:1019:GLU:O	2.53	0.41
1:A:1049:ILE:HG22	1:A:1184:PHE:CD2	2.56	0.41
2:D:54:VAL:HG21	2:D:796:LYS:HG3	2.01	0.41
2:D:71:GLU:HB3	2:D:630:TYR:CE1	2.55	0.41
2:D:517:PRO:HA	2:D:579:ILE:HG23	2.02	0.41
3:C:159:LYS:HA	3:C:159:LYS:HD2	1.74	0.41
3:C:193:THR:OG1	3:C:194:ASP:N	2.52	0.41
1:A:1596:MET:SD	1:A:1599:ASN:ND2	2.92	0.41
2:D:61:TYR:O	2:D:68:TYR:OH	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLN:HG2	3:C:254:ILE:HD12	2.03	0.41
1:A:150:ASP:OD1	1:A:150:ASP:O	2.38	0.41
2:D:730:LYS:HB2	2:D:730:LYS:HE2	1.85	0.41
3:C:62:PHE:CD1	3:C:173:VAL:HG11	2.56	0.41
1:A:135:PHE:O	1:A:139:VAL:HG23	2.21	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.91	0.41
1:A:928:PHE:O	1:A:952:ILE:HG13	2.21	0.41
1:A:1068:VAL:O	1:A:1072:LYS:HB3	2.21	0.41
1:A:1536:ILE:HG22	1:A:1537:LEU:H	1.86	0.41
1:A:1569:LEU:HD21	1:A:1581:LEU:O	2.21	0.41
8:A:2302:3PE:H352	8:A:2302:3PE:H282	2.03	0.41
2:D:73:ASN:N	2:D:628:PHE:O	2.53	0.41
2:D:76:ARG:NH1	2:D:585:GLU:OE1	2.54	0.41
2:D:77:GLN:H	2:D:77:GLN:HG2	1.62	0.41
2:D:362:THR:OG1	2:D:363:ASP:N	2.54	0.41
2:D:687:ILE:HA	2:D:687:ILE:HD12	1.80	0.41
2:D:782:LYS:NZ	2:D:782:LYS:HA	2.36	0.41
2:D:1021:LYS:HD3	2:D:1021:LYS:HA	1.84	0.41
3:C:104:TRP:CD1	3:C:120:SER:HB2	2.56	0.41
3:C:185:PRO:O	3:C:322:TYR:HB2	2.20	0.41
3:C:206:HIS:N	3:C:206:HIS:HD2	2.16	0.41
1:A:232:ASP:O	1:A:234:LYS:N	2.44	0.41
1:A:427:LYS:O	1:A:431:GLU:HB3	2.21	0.41
1:A:895:ARG:HG3	1:A:974:ALA:HB2	2.03	0.41
1:A:1001:LEU:HA	1:A:1001:LEU:HD12	1.87	0.41
1:A:1101:VAL:HG12	2:D:416:ILE:HD12	2.02	0.41
2:D:393:ASN:OD1	2:D:393:ASN:N	2.53	0.41
2:D:406:ASN:O	2:D:408:GLY:N	2.54	0.41
3:C:63:ALA:HB3	3:C:174:VAL:H	1.85	0.41
3:C:344:ASP:OD1	3:C:345:ALA:N	2.54	0.41
1:A:234:LYS:NZ	1:A:234:LYS:HB3	2.36	0.40
1:A:299:TYR:CE1	1:A:307:VAL:HG22	2.56	0.40
1:A:682:MET:HA	2:D:267:LEU:HD13	2.03	0.40
1:A:910:ILE:O	1:A:914:SER:OG	2.36	0.40
1:A:1003:SER:C	1:A:1005:GLY:N	2.75	0.40
1:A:1049:ILE:HD13	1:A:1181:PHE:HE1	1.87	0.40
1:A:1203:ASP:OD2	1:A:1206:GLN:HB2	2.21	0.40
9:A:2303:CLR:H213	9:A:2303:CLR:H231	1.83	0.40
2:D:37:VAL:HG11	2:D:1006:GLU:HG2	2.03	0.40
2:D:781:ASN:CG	2:D:782:LYS:H	2.25	0.40
2:D:848:MET:O	2:D:1020:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:849:ASP:HA	2:D:863:ASN:HD21	1.86	0.40
1:A:126:PHE:O	1:A:126:PHE:CG	2.72	0.40
1:A:304:ILE:HB	1:A:305:ALA:H	1.59	0.40
1:A:583:TYR:CE1	1:A:589:ASN:HB3	2.57	0.40
1:A:1560:ILE:HG12	1:A:1604:VAL:H	1.86	0.40
2:D:461:THR:HG22	2:D:462:GLY:O	2.22	0.40
2:D:205:TRP:NE1	2:D:456:LEU:HD22	2.35	0.40
2:D:333:TYR:HE2	2:D:360:LEU:HD21	1.86	0.40
2:D:566:LEU:HD23	2:D:566:LEU:HA	1.85	0.40
1:A:618:VAL:HG11	1:A:1065:CYS:HB2	2.03	0.40
1:A:1569:LEU:HB2	1:A:1578:PHE:HB3	2.04	0.40
2:D:662:ALA:HA	2:D:663:PRO:HD3	1.89	0.40
3:C:58:LYS:HA	3:C:59:PRO:HD3	1.96	0.40
3:C:122:GLN:OE1	3:C:122:GLN:N	2.54	0.40
3:C:175:PRO:HG3	3:C:257:ILE:HG22	2.03	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	1244/2201 (56%)	1117 (90%)	103 (8%)	24 (2%)	8 36
2	D	936/1103 (85%)	857 (92%)	74 (8%)	5 (0%)	29 68
3	C	322/484 (66%)	263 (82%)	52 (16%)	7 (2%)	6 31
All	All	2502/3788 (66%)	2237 (89%)	229 (9%)	36 (1%)	15 43

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ILE
1	A	123	TRP

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Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1011	ILE
1	A	1013	VAL
1	A	1550	ALA
1	A	1554	PRO
1	A	1568	LEU
2	D	781	ASN
3	C	140	ASN
3	C	203	PHE
1	A	122	GLU
1	A	1008	SER
1	A	1016	ILE
1	A	1022	VAL
1	A	1551	GLU
1	A	1599	ASN
1	A	1606	PHE
1	A	304	ILE
1	A	1002	ILE
2	D	220	ALA
3	C	136	ARG
3	C	211	ARG
3	C	315	LEU
1	A	1019	VAL
2	D	782	LYS
2	D	785	PRO
3	C	326	VAL
1	A	1012	ASN
3	C	267	VAL
1	A	119	SER
1	A	1581	LEU
1	A	124	LYS
1	A	1586	VAL
1	A	1575	PRO
2	D	219	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	1117/1896 (59%)	977 (88%)	140 (12%)	4 20
2	D	837/971 (86%)	765 (91%)	72 (9%)	10 37
3	C	287/426 (67%)	252 (88%)	35 (12%)	5 21
All	All	2241/3293 (68%)	1994 (89%)	247 (11%)	10 25

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ILE
1	A	121	VAL
1	A	124	LYS
1	A	126	PHE
1	A	137	ASN
1	A	152	SER
1	A	171	THR
1	A	208	PHE
1	A	212	LEU
1	A	213	GLU
1	A	217	LYS
1	A	234	LYS
1	A	236	LEU
1	A	304	ILE
1	A	310	GLU
1	A	322	HIS
1	A	330	THR
1	A	337	ASP
1	A	360	ILE
1	A	379	ASP
1	A	405	SER
1	A	412	ARG
1	A	413	GLU
1	A	416	LYS
1	A	428	GLN
1	A	431	GLU
1	A	432	GLU
1	A	438	LEU
1	A	440	TRP
1	A	442	THR
1	A	512	PHE
1	A	518	ARG
1	A	526	PHE
1	A	539	LEU

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Mol	Chain	Res	Type
1	A	550	ASN
1	A	553	THR
1	A	561	LYS
1	A	571	MET
1	A	580	LEU
1	A	583	TYR
1	A	588	PHE
1	A	590	ARG
1	A	593	CYS
1	A	595	VAL
1	A	609	LYS
1	A	610	ILE
1	A	611	MET
1	A	614	LEU
1	A	618	VAL
1	A	647	SER
1	A	649	ARG
1	A	660	LEU
1	A	687	SER
1	A	746	ASN
1	A	764	SER
1	A	768	GLU
1	A	770	GLU
1	A	775	ARG
1	A	778	LEU
1	A	780	ARG
1	A	904	ASN
1	A	912	LEU
1	A	914	SER
1	A	916	SER
1	A	928	PHE
1	A	960	PHE
1	A	972	MET
1	A	986	ARG
1	A	994	LEU
1	A	999	VAL
1	A	1001	LEU
1	A	1002	ILE
1	A	1004	PHE
1	A	1007	GLN
1	A	1014	VAL
1	A	1015	LYS

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Mol	Chain	Res	Type
1	A	1016	ILE
1	A	1017	LEU
1	A	1042	VAL
1	A	1051	ASN
1	A	1075	LEU
1	A	1079	SER
1	A	1126	MET
1	A	1139	GLU
1	A	1160	VAL
1	A	1184	PHE
1	A	1199	ASN
1	A	1207	ARG
1	A	1217	ARG
1	A	1219	LEU
1	A	1255	CYS
1	A	1263	GLN
1	A	1274	LEU
1	A	1284	VAL
1	A	1306	PHE
1	A	1308	PHE
1	A	1372	SER
1	A	1386	LYS
1	A	1390	ARG
1	A	1392	GLU
1	A	1408	LEU
1	A	1449	THR
1	A	1474	MET
1	A	1493	THR
1	A	1495	CYS
1	A	1527	PHE
1	A	1531	THR
1	A	1532	ARG
1	A	1537	LEU
1	A	1540	HIS
1	A	1546	LYS
1	A	1547	ARG
1	A	1548	ILE
1	A	1563	LEU
1	A	1564	ASP
1	A	1565	VAL
1	A	1568	LEU
1	A	1569	LEU

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Mol	Chain	Res	Type
1	A	1570	ARG
1	A	1571	ARG
1	A	1572	ILE
1	A	1573	GLN
1	A	1576	LEU
1	A	1578	PHE
1	A	1581	LEU
1	A	1582	CYS
1	A	1586	VAL
1	A	1588	CYS
1	A	1599	ASN
1	A	1603	THR
1	A	1604	VAL
1	A	1605	MET
1	A	1610	LEU
1	A	1618	LEU
1	A	1623	GLU
1	A	1631	GLU
1	A	1636	ILE
1	A	1638	LYS
1	A	1646	MET
1	A	1649	LEU
2	D	31	VAL
2	D	32	THR
2	D	39	LYS
2	D	44	LEU
2	D	66	ASP
2	D	91	SER
2	D	142	SER
2	D	144	ARG
2	D	160	SER
2	D	176	SER
2	D	187	SER
2	D	193	PHE
2	D	203	LEU
2	D	210	SER
2	D	250	SER
2	D	252	LYS
2	D	286	ASP
2	D	295	ASN
2	D	316	LYS
2	D	335	LYS

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Mol	Chain	Res	Type
2	D	337	PHE
2	D	366	GLU
2	D	371	GLU
2	D	379	ASP
2	D	393	ASN
2	D	439	ASP
2	D	478	ASN
2	D	481	ASN
2	D	500	LEU
2	D	507	CYS
2	D	522	LEU
2	D	530	LYS
2	D	532	ILE
2	D	587	THR
2	D	590	THR
2	D	618	SER
2	D	631	ILE
2	D	670	LEU
2	D	685	GLU
2	D	686	PHE
2	D	689	ARG
2	D	691	THR
2	D	704	ARG
2	D	719	TYR
2	D	724	LYS
2	D	743	VAL
2	D	746	LYS
2	D	750	GLU
2	D	781	ASN
2	D	782	LYS
2	D	783	SER
2	D	795	SER
2	D	845	SER
2	D	846	ASP
2	D	854	ASP
2	D	873	ARG
2	D	897	SER
2	D	899	ASP
2	D	903	VAL
2	D	984	ASP
2	D	985	ASN
2	D	986	ASP

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Mol	Chain	Res	Type
2	D	989	SER
2	D	995	ASP
2	D	1000	SER
2	D	1003	PHE
2	D	1026	CYS
2	D	1028	THR
2	D	1037	THR
2	D	1053	ARG
2	D	1067	ASP
2	D	1069	THR
3	C	41	ARG
3	C	42	ARG
3	C	50	GLN
3	C	65	ARG
3	C	75	ASP
3	C	83	SER
3	C	94	HIS
3	C	96	LYS
3	C	105	ILE
3	C	110	LYS
3	C	134	LYS
3	C	163	LYS
3	C	177	MET
3	C	188	LYS
3	C	200	LEU
3	C	201	PHE
3	C	204	LEU
3	C	205	LYS
3	C	206	HIS
3	C	207	ARG
3	C	208	PHE
3	C	211	ARG
3	C	220	ASP
3	C	225	LYS
3	C	282	LYS
3	C	283	THR
3	C	307	ARG
3	C	312	MET
3	C	313	LYS
3	C	320	MET
3	C	322	TYR
3	C	324	LYS

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Mol	Chain	Res	Type
3	C	325	LEU
3	C	331	GLU
3	C	333	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	393	ASN
2	D	482	GLN
2	D	717	GLN
3	C	50	GLN
3	C	206	HIS
3	C	265	GLN
3	C	276	HIS

5.3.3 RNA (i)

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)

13 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	B	1	4,2	14,14,15	0.87	1 (7%)	17,19,21	1.37	1 (5%)
4	NAG	B	2	4	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	B	3	4	14,14,15	0.33	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	E	1	2,5	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	0.35	0
6	NAG	F	1	6,2	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	F	2	6	14,14,15	0.21	0	17,19,21	0.42	0
6	NAG	F	3	6	14,14,15	0.98	1 (7%)	17,19,21	1.64	2 (11%)
6	NAG	F	4	6	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
5	NAG	G	1	2,5	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	G	2	5	14,14,15	0.29	0	17,19,21	0.43	0
5	NAG	H	1	2,5	14,14,15	0.46	0	17,19,21	0.36	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.44	0

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	B	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	NAG	B	3	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	F	3	6	-	5/6/23/26	0/1/1/1
6	NAG	F	4	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.20	1.48	1.43
4	B	1	NAG	O5-C1	3.16	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1	NAG	C1-O5-C5	5.41	119.53	112.19
6	F	3	NAG	C1-O5-C5	4.42	118.18	112.19
6	F	3	NAG	C2-N2-C7	4.35	129.09	122.90
6	F	4	NAG	C2-N2-C7	4.32	129.05	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	3	NAG	C4-C5-C6-O6
6	F	3	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
4	B	3	NAG	C8-C7-N2-C2
4	B	3	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
6	F	3	NAG	C8-C7-N2-C2
6	F	3	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
6	F	1	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
6	F	4	NAG	C4-C5-C6-O6
6	F	4	NAG	O5-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
5	G	1	NAG	O5-C5-C6-O6
6	F	3	NAG	C3-C2-N2-C7
6	F	4	NAG	C3-C2-N2-C7

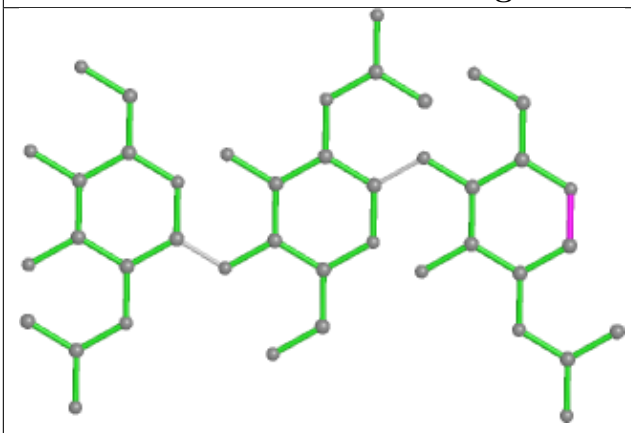
There are no ring outliers.

3 monomers are involved in 3 short contacts:

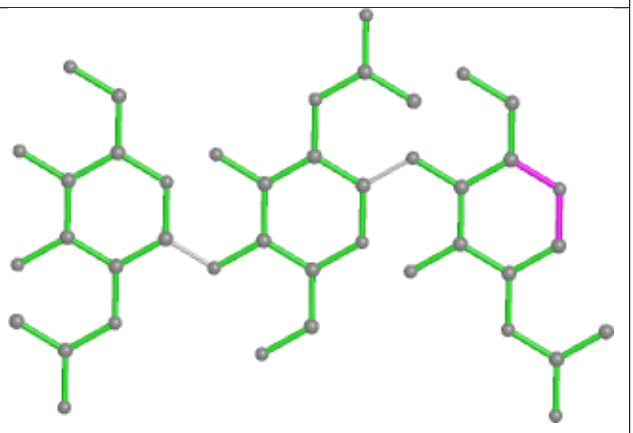
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	4	NAG	1	0
6	F	1	NAG	1	0
6	F	3	NAG	1	0

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

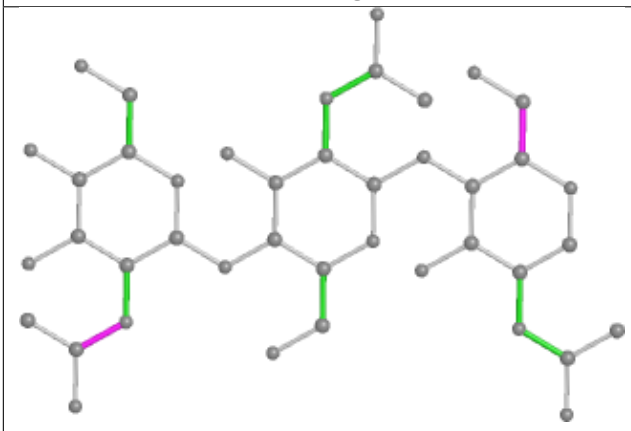
Oligosaccharide Chain B



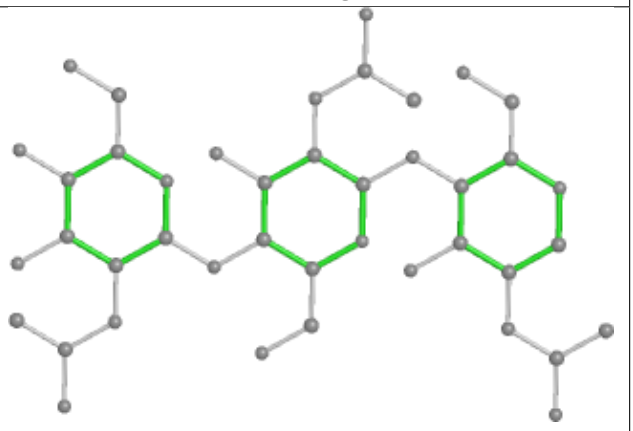
Bond lengths



Bond angles

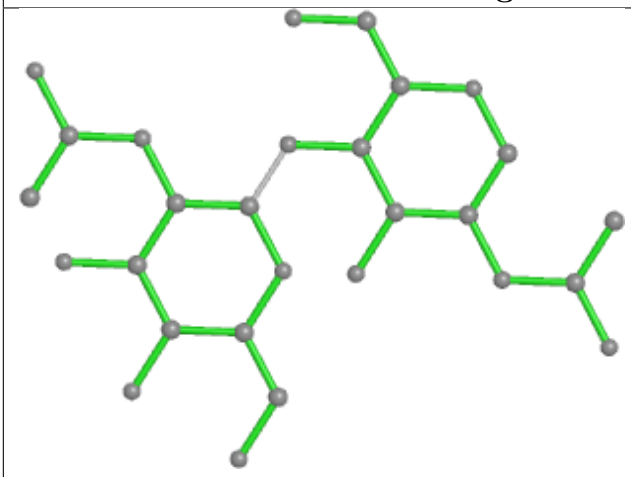


Torsions

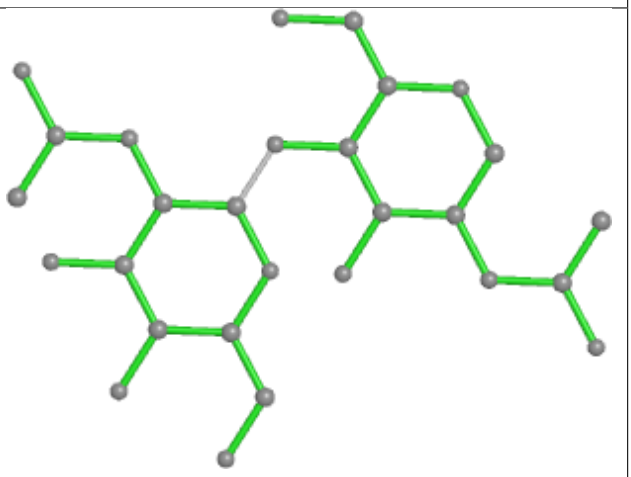


Rings

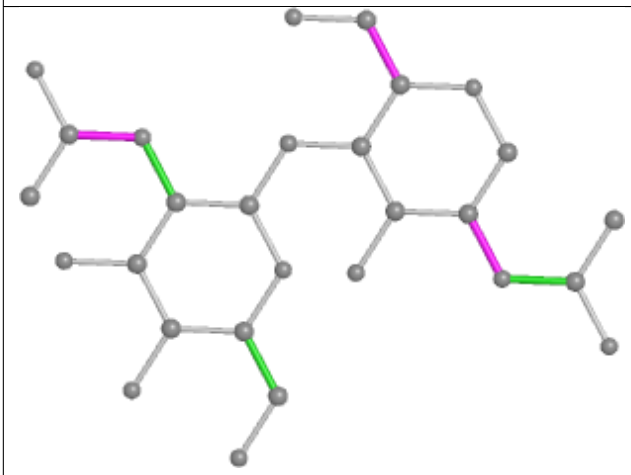
Oligosaccharide Chain E



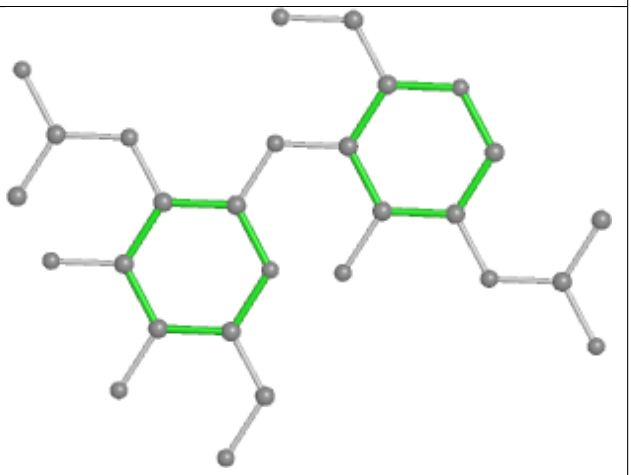
Bond lengths



Bond angles

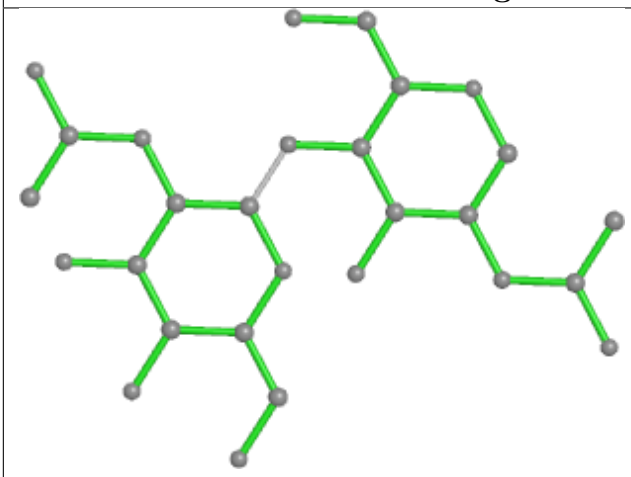


Torsions

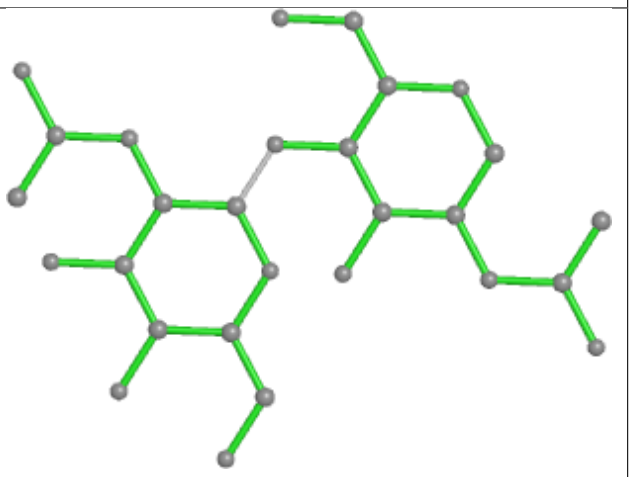


Rings

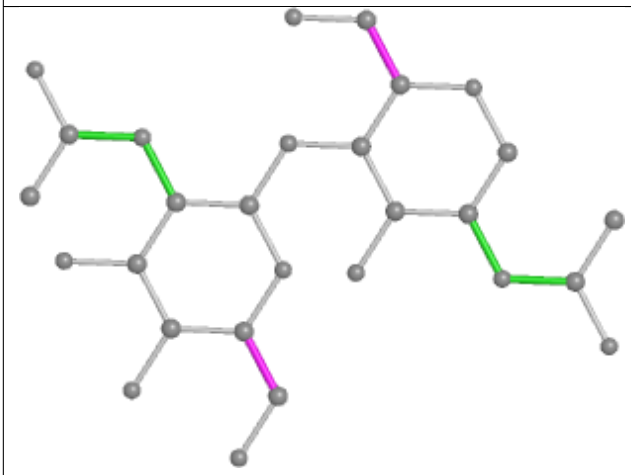
Oligosaccharide Chain G



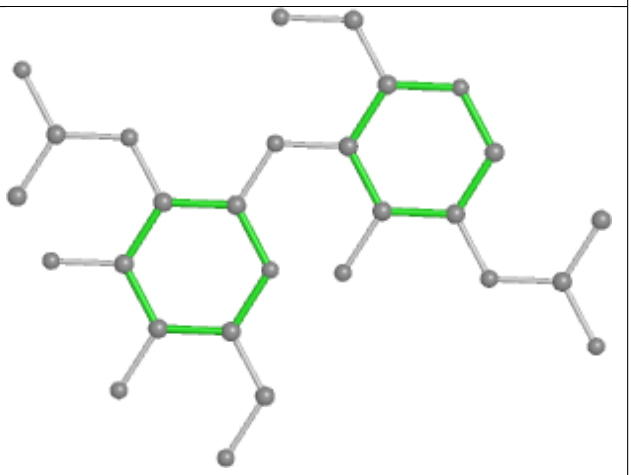
Bond lengths



Bond angles

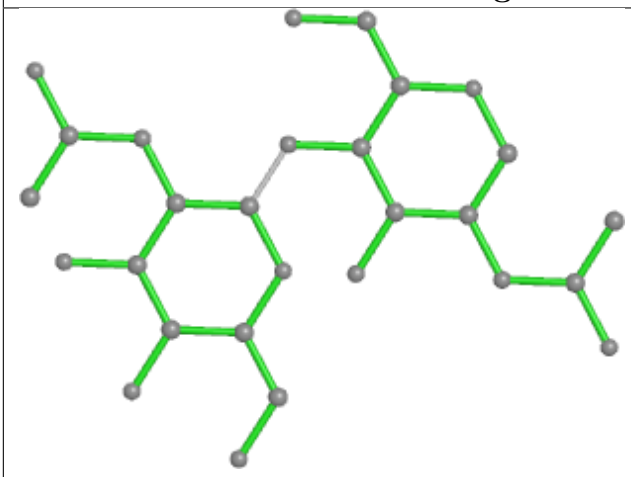


Torsions

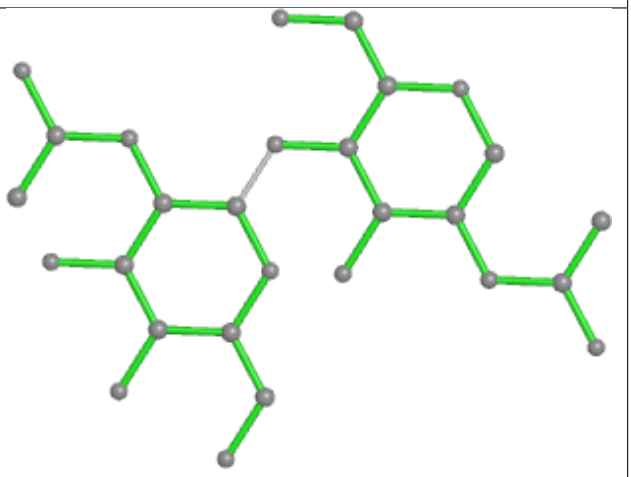


Rings

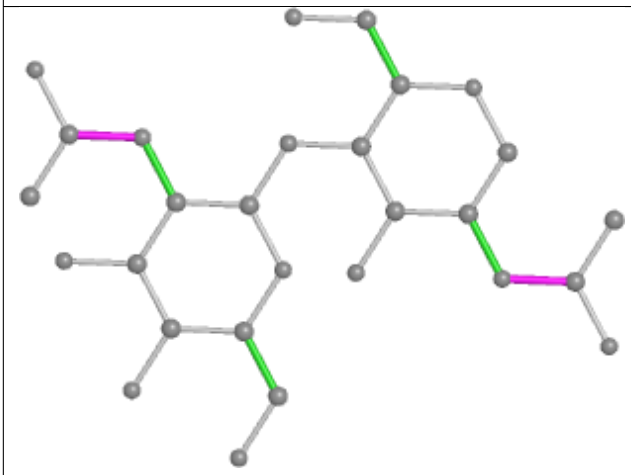
Oligosaccharide Chain H



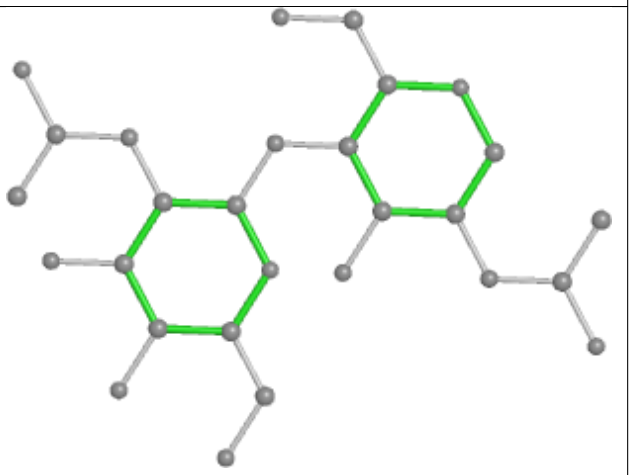
Bond lengths



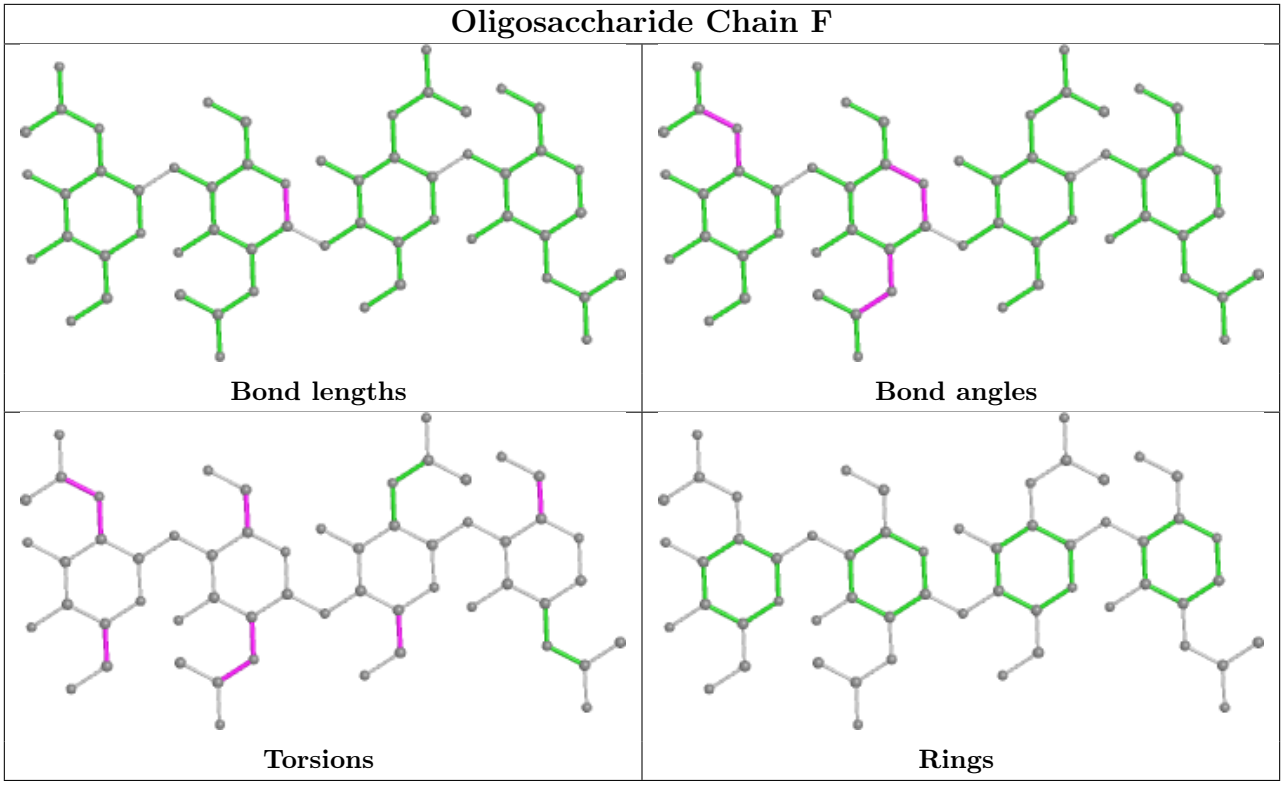
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
10	NAG	D	1203	2	14,14,15	0.79	1 (7%)	17,19,21	0.63	0
9	CLR	A	2303	-	31,31,31	0.36	0	48,48,48	0.66	0
9	CLR	A	2304	-	31,31,31	0.39	0	48,48,48	0.68	0
8	3PE	A	2302	-	39,39,50	0.57	0	42,44,55	0.68	2 (4%)
10	NAG	D	1202	2	14,14,15	0.46	0	17,19,21	0.39	0
11	PT5	A	2307	-	63,63,69	1.36	7 (11%)	76,81,87	1.16	5 (6%)
10	NAG	A	2306	1	14,14,15	0.38	0	17,19,21	1.27	1 (5%)
9	CLR	A	2305	-	31,31,31	0.36	0	48,48,48	0.51	0

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
10	NAG	D	1203	2	-	0/6/23/26	0/1/1/1
9	CLR	A	2303	-	-	7/10/68/68	0/4/4/4
9	CLR	A	2304	-	-	7/10/68/68	0/4/4/4
8	3PE	A	2302	-	-	15/43/43/54	-
10	NAG	D	1202	2	-	4/6/23/26	0/1/1/1
11	PT5	A	2307	-	-	23/60/84/90	0/1/1/1
10	NAG	A	2306	1	-	2/6/23/26	0/1/1/1
9	CLR	A	2305	-	-	8/10/68/68	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2307	PT5	P4-O4	3.85	1.66	1.59
11	A	2307	PT5	P5-O5	3.59	1.66	1.59
11	A	2307	PT5	O18-C11	3.51	1.43	1.33
11	A	2307	PT5	O16-C8	-2.81	1.39	1.46
11	A	2307	PT5	P1-O1	2.78	1.67	1.60
11	A	2307	PT5	C31-C11	2.65	1.58	1.50
11	A	2307	PT5	O16-C10	2.54	1.41	1.34
10	D	1203	NAG	C1-C2	2.42	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2306	NAG	C1-O5-C5	4.76	118.64	112.19
11	A	2307	PT5	O16-C10-C12	3.65	119.37	111.50
11	A	2307	PT5	C20-C19-C18	3.46	152.74	123.57
11	A	2307	PT5	C17-C16-C15	3.41	152.31	123.57
11	A	2307	PT5	O18-C11-C31	2.62	120.12	111.91
8	A	2302	3PE	C2-O21-C21	2.47	123.88	117.79
8	A	2302	3PE	O12-P-O14	2.34	123.81	112.24
11	A	2307	PT5	C12-C13-C14	-2.24	109.23	113.23

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2302	3PE	O13-C11-C12-N
9	A	2303	CLR	C13-C17-C20-C21
9	A	2303	CLR	C16-C17-C20-C22
9	A	2304	CLR	C13-C17-C20-C21
9	A	2304	CLR	C13-C17-C20-C22
9	A	2304	CLR	C16-C17-C20-C22
11	A	2307	PT5	C1-O1-P1-O13
11	A	2307	PT5	C8-C7-O13-P1
11	A	2307	PT5	C5-O5-P5-O52
9	A	2303	CLR	C16-C17-C20-C21
9	A	2304	CLR	C16-C17-C20-C21
9	A	2303	CLR	C13-C17-C20-C22
10	D	1202	NAG	C4-C5-C6-O6
9	A	2304	CLR	C21-C20-C22-C23
10	A	2306	NAG	C4-C5-C6-O6
8	A	2302	3PE	C32-C31-O31-C3
10	D	1202	NAG	O5-C5-C6-O6
8	A	2302	3PE	O32-C31-O31-C3
9	A	2303	CLR	C21-C20-C22-C23
10	A	2306	NAG	O5-C5-C6-O6
9	A	2305	CLR	C17-C20-C22-C23
8	A	2302	3PE	C22-C21-O21-C2
11	A	2307	PT5	C31-C11-O18-C9
10	D	1202	NAG	C8-C7-N2-C2
10	D	1202	NAG	O7-C7-N2-C2
9	A	2305	CLR	C21-C20-C22-C23
9	A	2304	CLR	C17-C20-C22-C23
9	A	2303	CLR	C20-C22-C23-C24
9	A	2303	CLR	C17-C20-C22-C23
8	A	2302	3PE	O22-C21-O21-C2
11	A	2307	PT5	O19-C11-O18-C9
11	A	2307	PT5	C7-O13-P1-O1
11	A	2307	PT5	C12-C13-C14-C15
8	A	2302	3PE	C1-C2-O21-C21
11	A	2307	PT5	C35-C36-C37-C38
11	A	2307	PT5	C37-C38-C39-C40
8	A	2302	3PE	C25-C26-C27-C28
11	A	2307	PT5	C34-C35-C36-C37
9	A	2305	CLR	C22-C23-C24-C25
11	A	2307	PT5	C10-C12-C13-C14
11	A	2307	PT5	C36-C37-C38-C39
11	A	2307	PT5	O13-C7-C8-C9
8	A	2302	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
11	A	2307	PT5	C39-C40-C41-C42
8	A	2302	3PE	O11-C1-C2-C3
11	A	2307	PT5	C15-C16-C17-C18
9	A	2305	CLR	C16-C17-C20-C22
9	A	2305	CLR	C13-C17-C20-C22
8	A	2302	3PE	C26-C27-C28-C29
9	A	2305	CLR	C16-C17-C20-C21
9	A	2305	CLR	C13-C17-C20-C21
8	A	2302	3PE	C22-C23-C24-C25
11	A	2307	PT5	O13-C7-C8-O16
11	A	2307	PT5	C5-O5-P5-O51
11	A	2307	PT5	C7-O13-P1-O12
11	A	2307	PT5	C31-C32-C33-C34
8	A	2302	3PE	O11-C1-C2-O21
11	A	2307	PT5	C40-C41-C42-C43
8	A	2302	3PE	C1-O11-P-O13
9	A	2305	CLR	C20-C22-C23-C24
11	A	2307	PT5	O17-C10-O16-C8
9	A	2304	CLR	C23-C24-C25-C26
11	A	2307	PT5	C12-C10-O16-C8
11	A	2307	PT5	C38-C39-C40-C41
8	A	2302	3PE	C1-O11-P-O14
8	A	2302	3PE	C31-C32-C33-C34

There are no ring outliers.

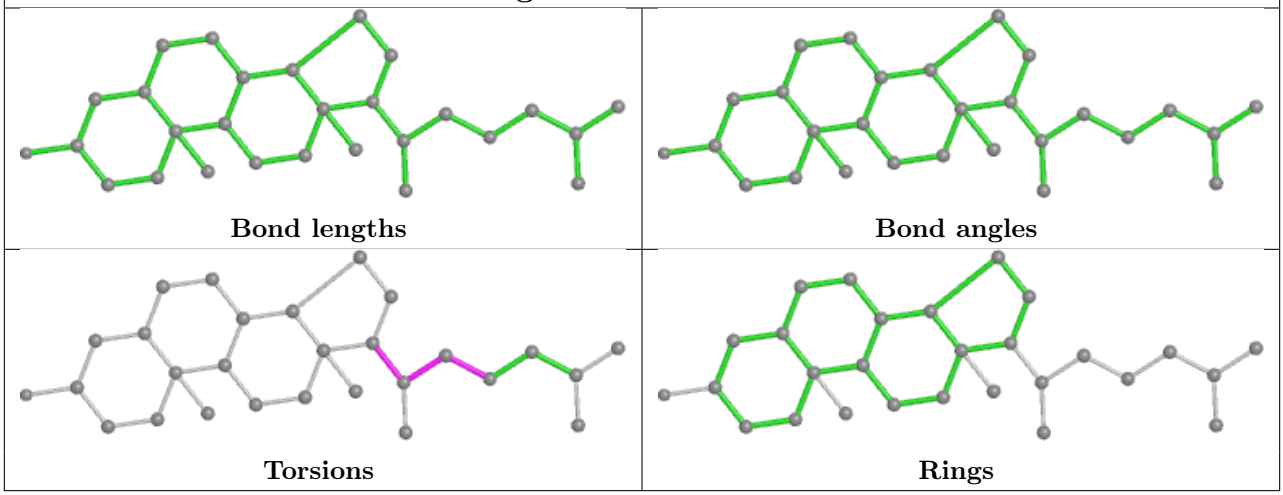
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2303	CLR	2	0
9	A	2304	CLR	3	0
8	A	2302	3PE	1	0
11	A	2307	PT5	2	0

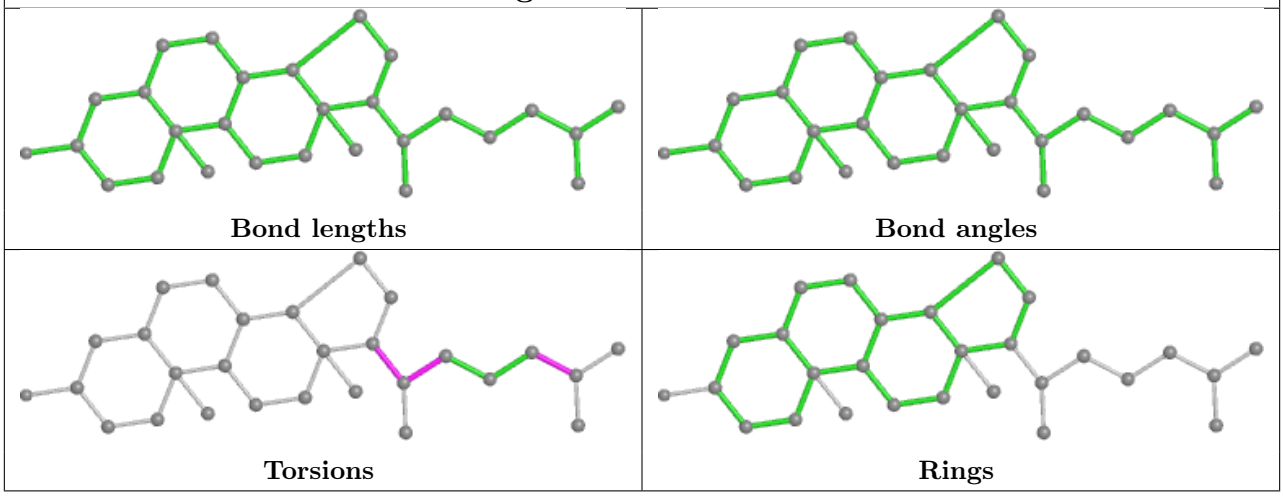
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

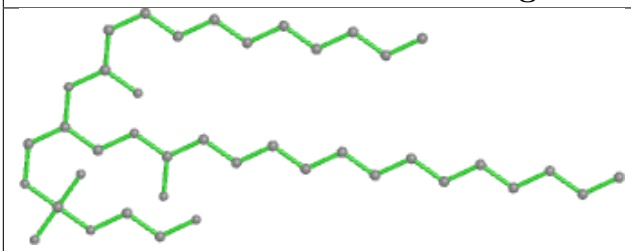
Ligand CLR A 2303



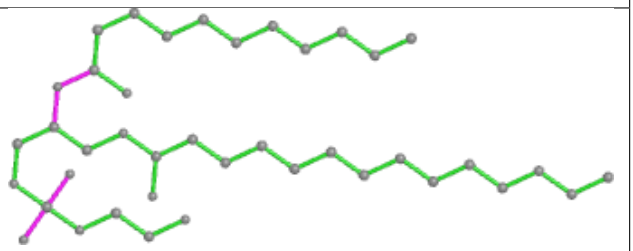
Ligand CLR A 2304



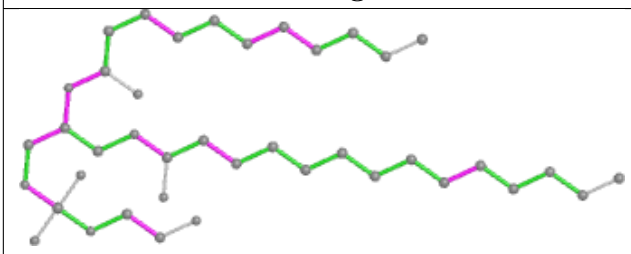
Ligand 3PE A 2302



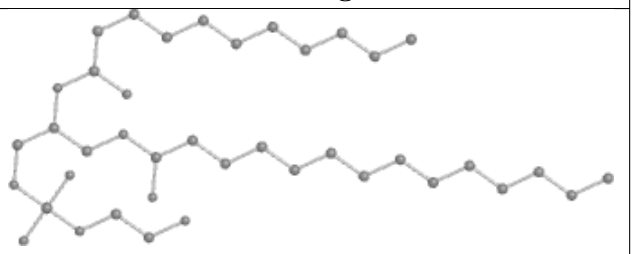
Bond lengths



Bond angles

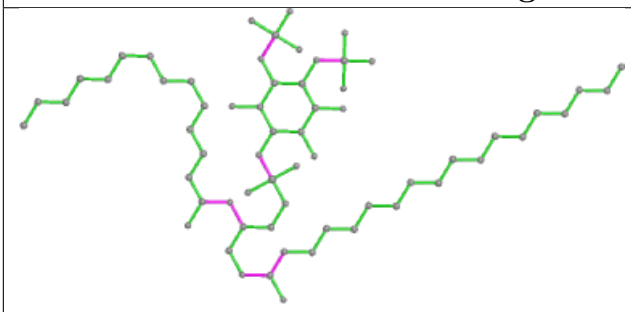


Torsions

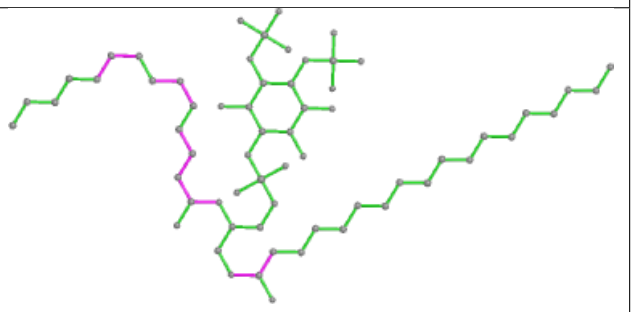


Rings

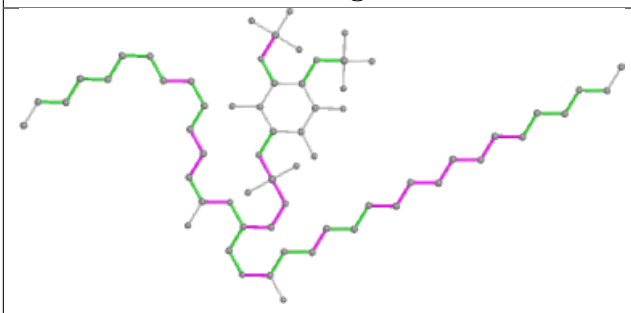
Ligand PT5 A 2307



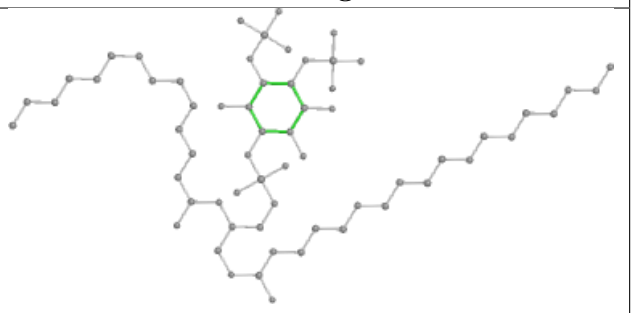
Bond lengths



Bond angles

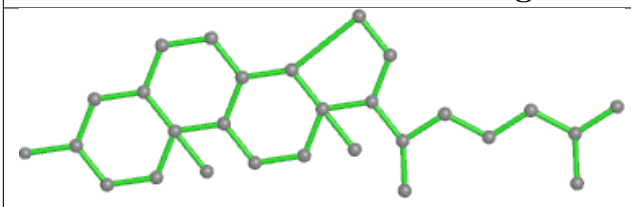


Torsions

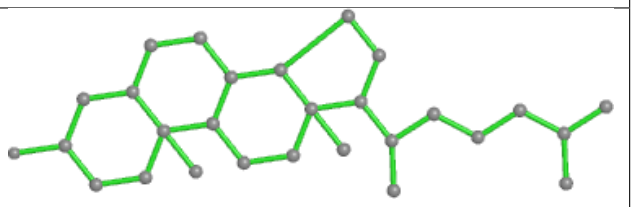


Rings

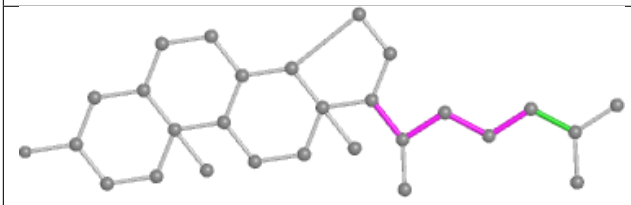
Ligand CLR A 2305



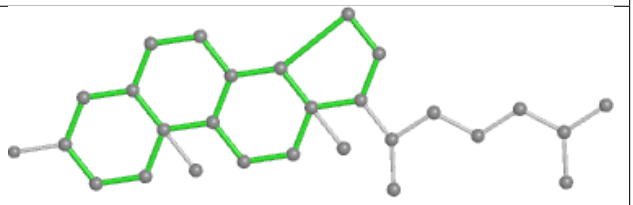
Bond lengths



Bond angles



Torsions



Rings

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.

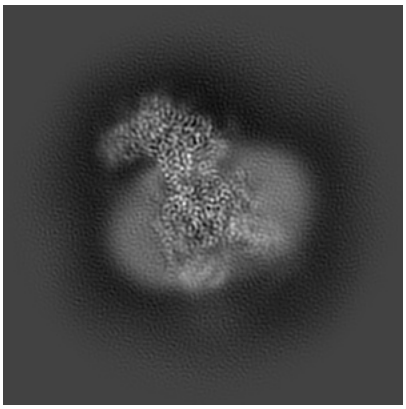
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37475. These allow visual inspection of the internal detail of the map and identification of artifacts.

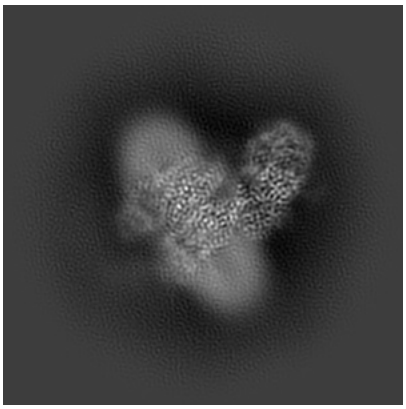
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

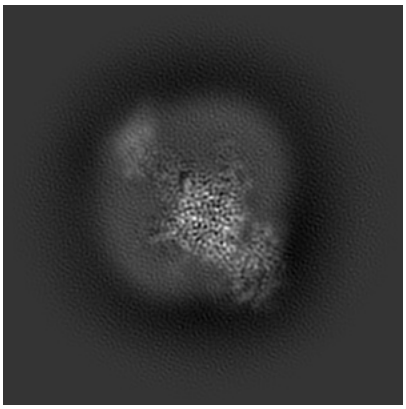
6.1.1 Primary map



X

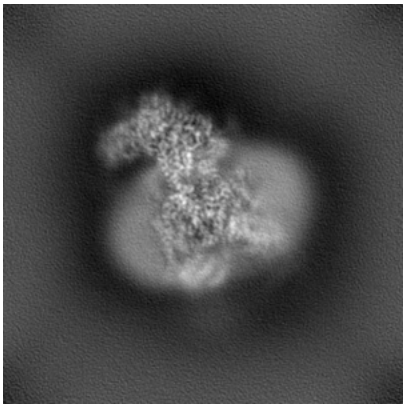


Y

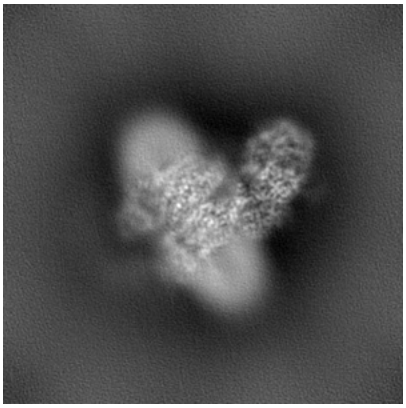


Z

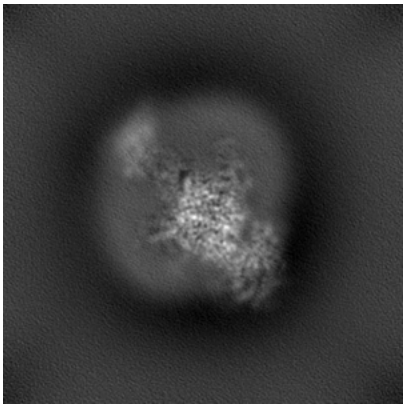
6.1.2 Raw map



X



Y

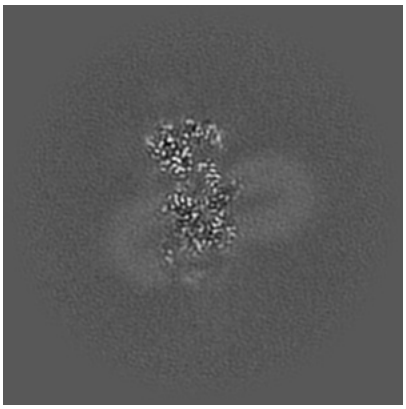


Z

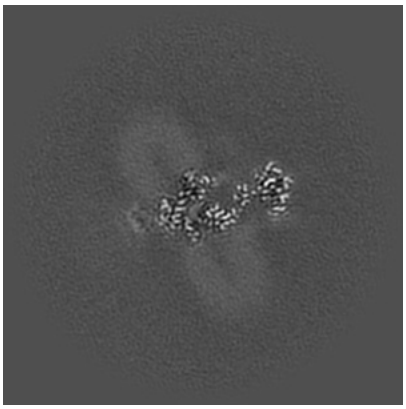
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

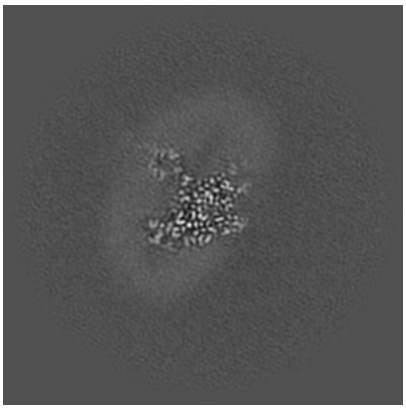
6.2.1 Primary map



X Index: 140

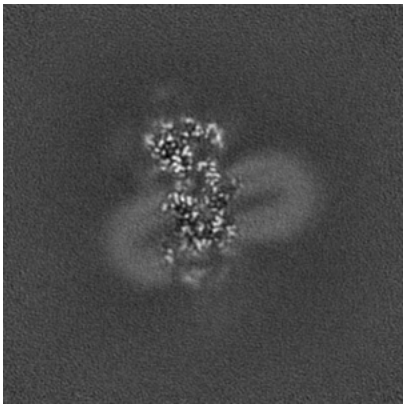


Y Index: 140

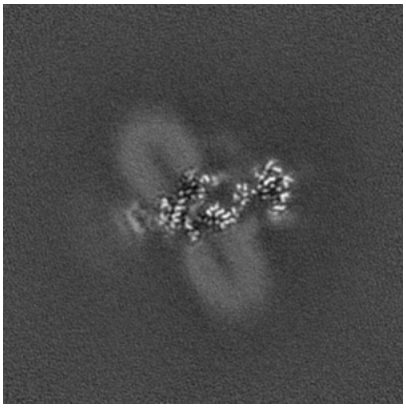


Z Index: 140

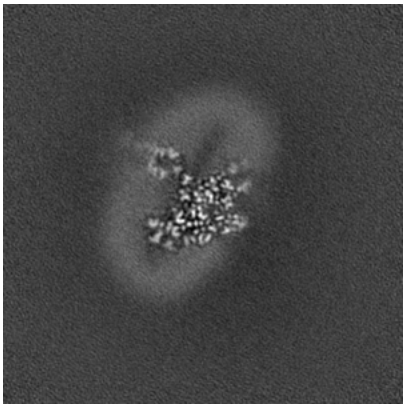
6.2.2 Raw map



X Index: 140



Y Index: 140

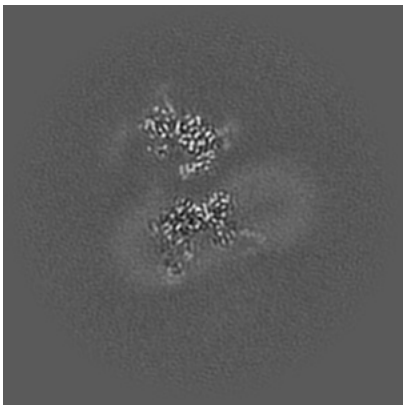


Z Index: 140

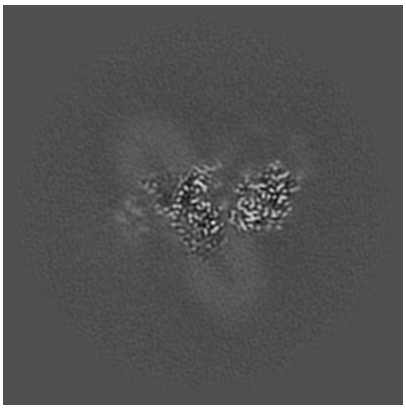
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

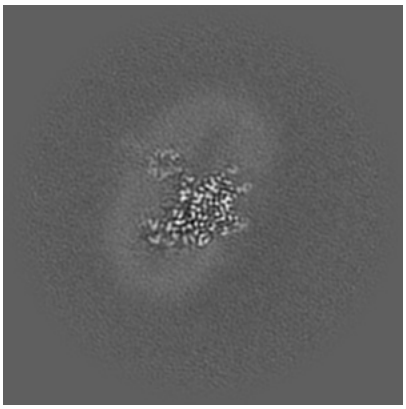
6.3.1 Primary map



X Index: 149

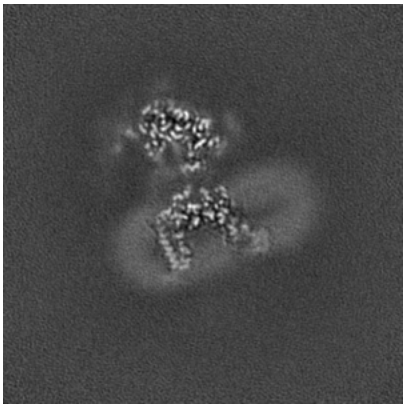


Y Index: 130

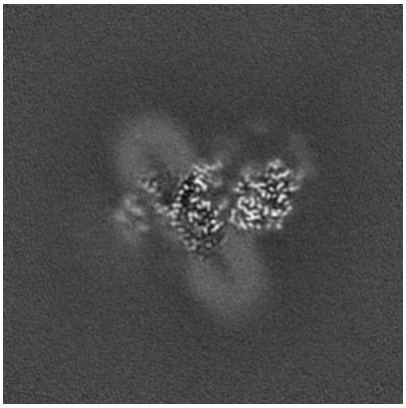


Z Index: 139

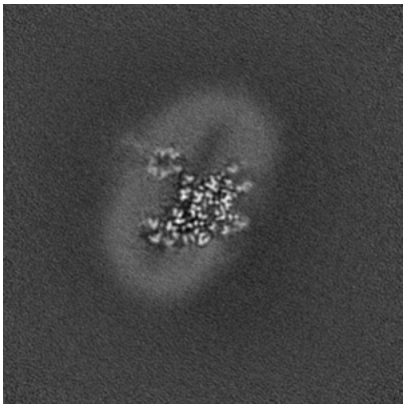
6.3.2 Raw map



X Index: 154



Y Index: 130

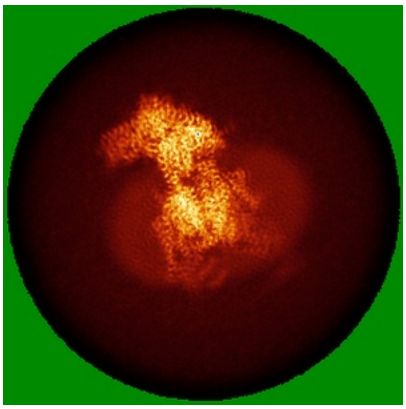


Z Index: 139

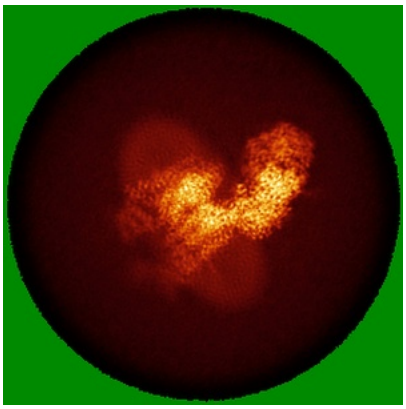
The images above show the largest variance slices of the map in three orthogonal directions.

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

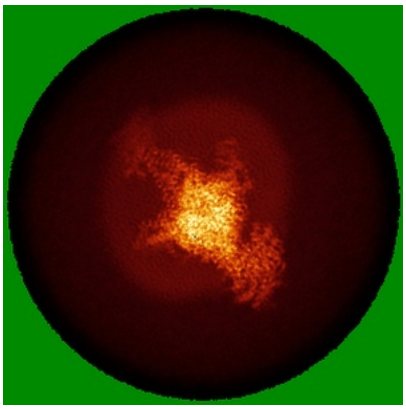
6.4.1 Primary map



X

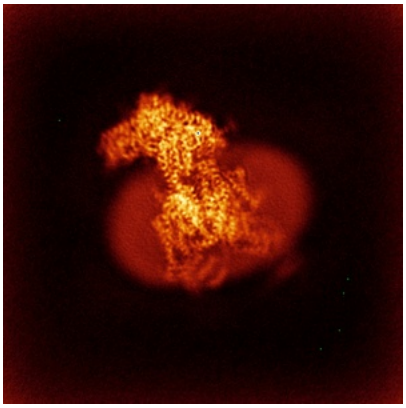


Y

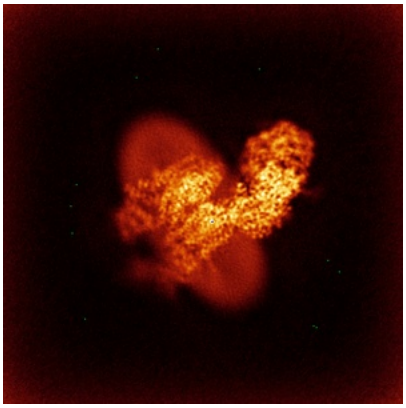


Z

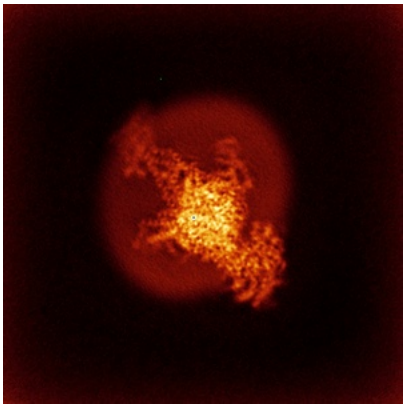
6.4.2 Raw map



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 0.35. 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.

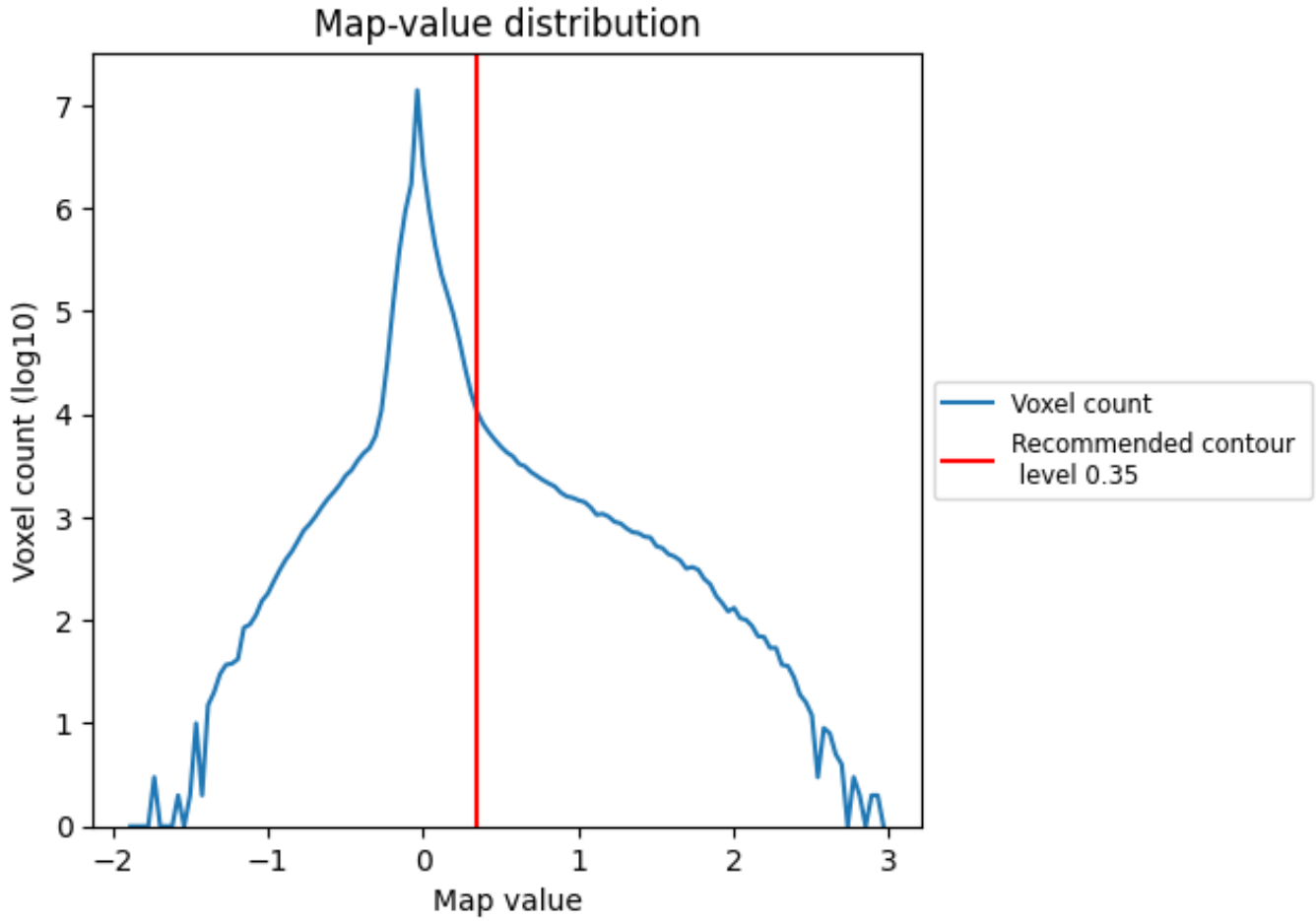
6.6 Mask visualisation (i)

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

7 Map analysis

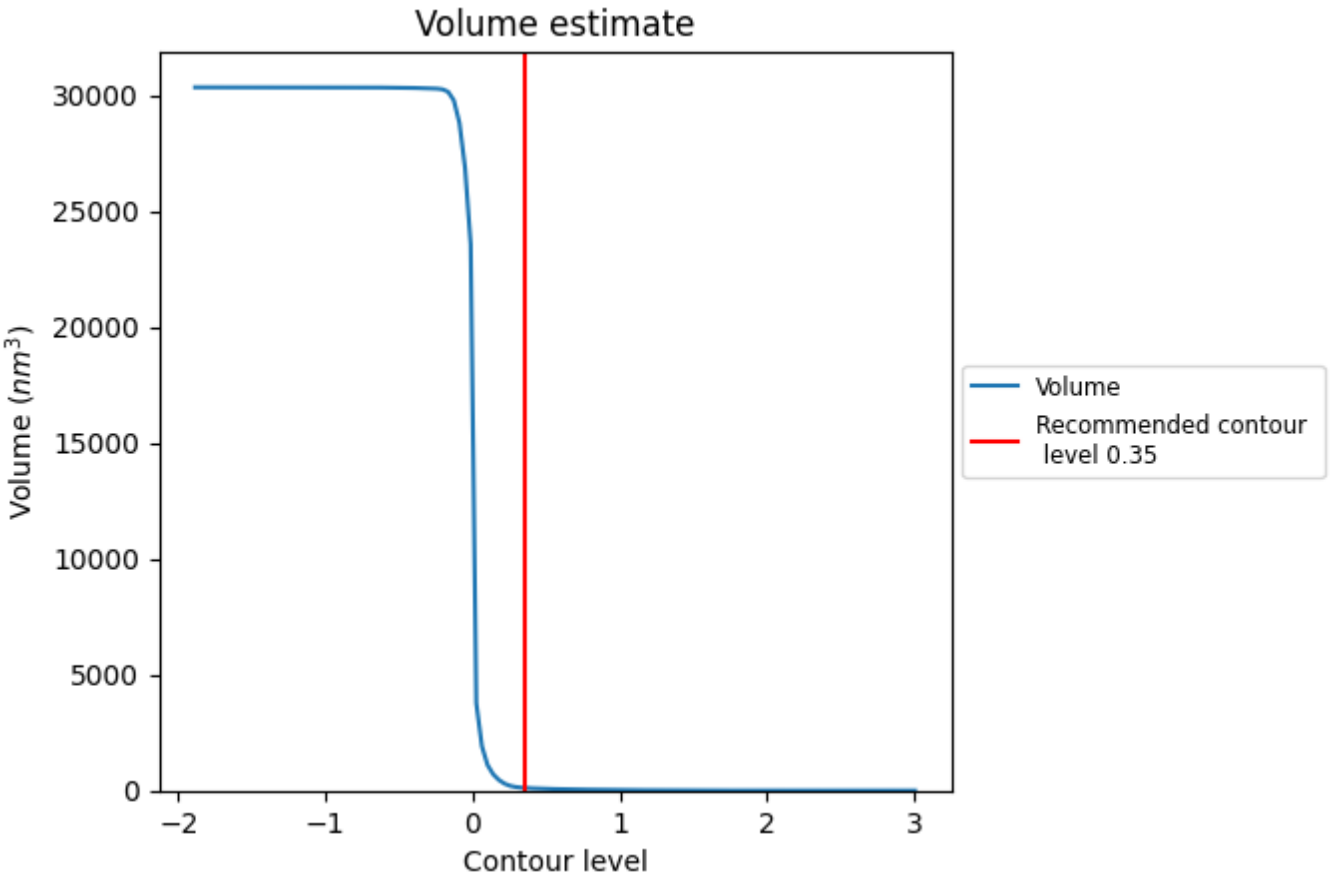
This section contains the results of statistical analysis of the map.

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.

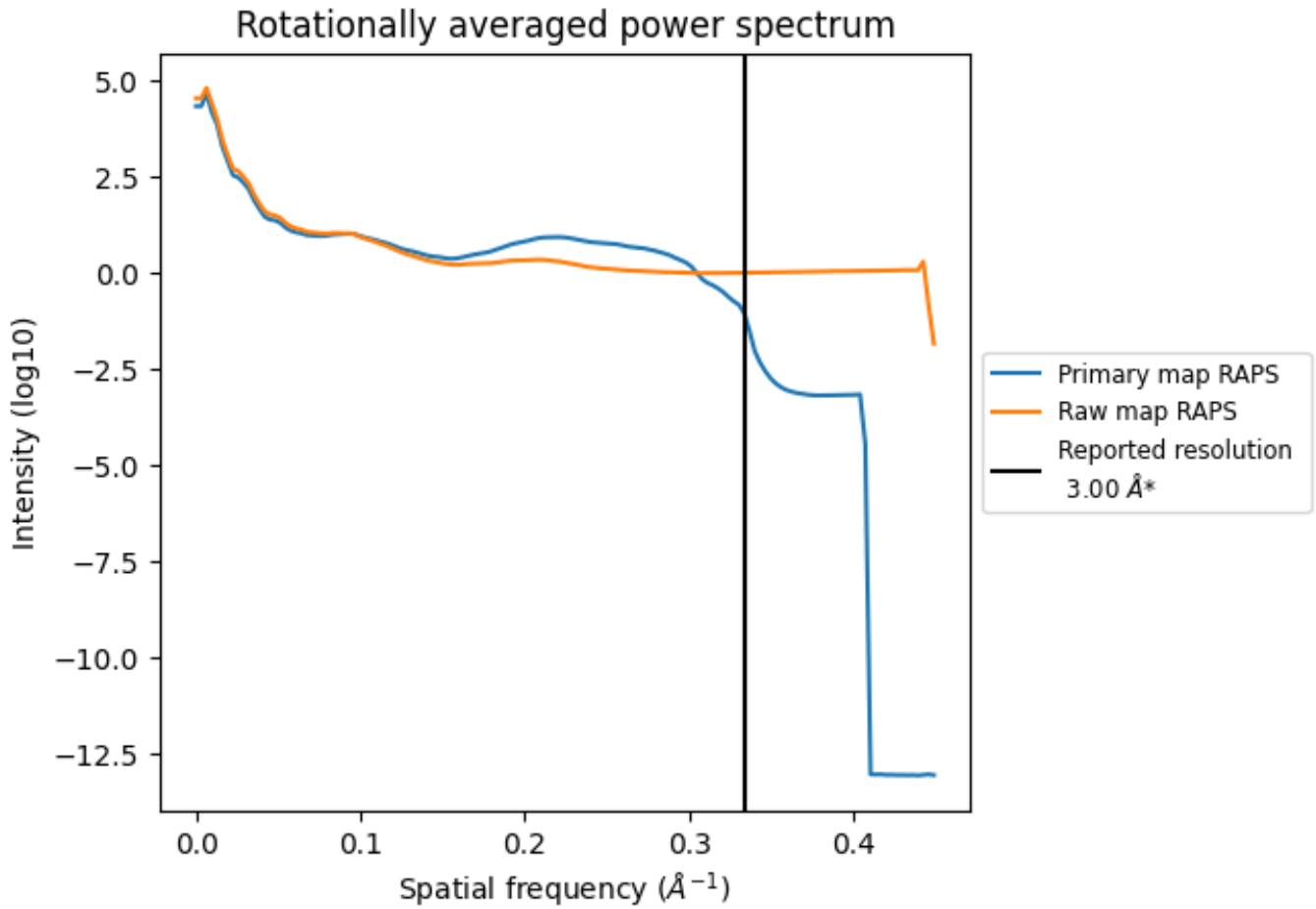
7.2 Volume estimate



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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)

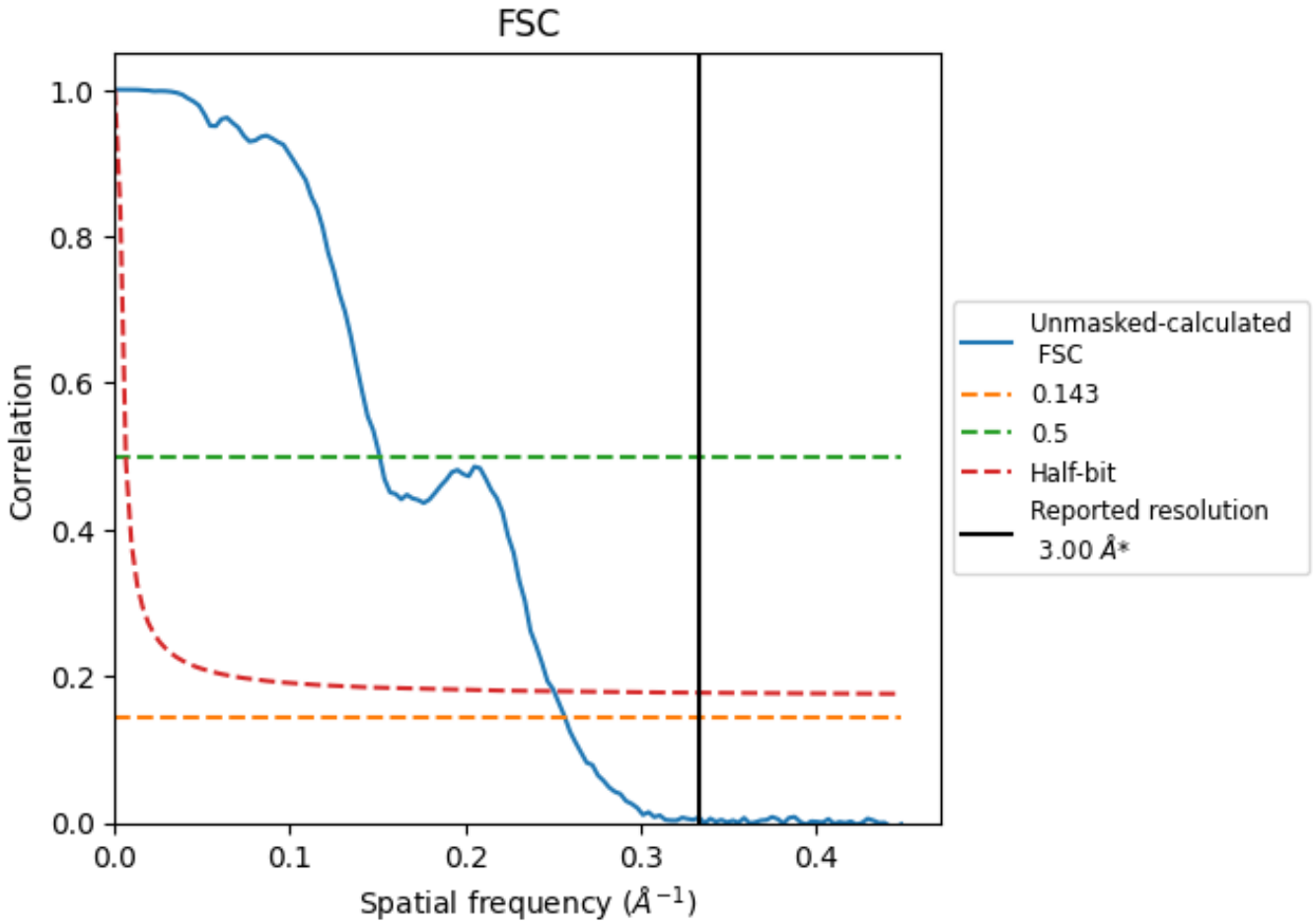


*Reported resolution corresponds to spatial frequency of 0.333 $Å^{-1}$

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)

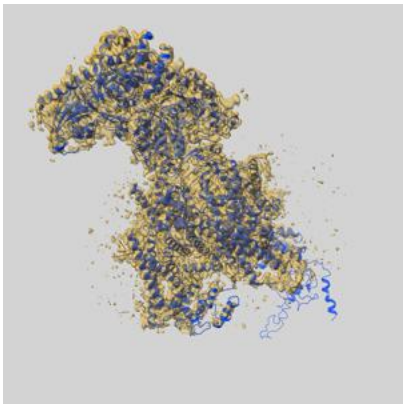
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	6.62	3.99

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

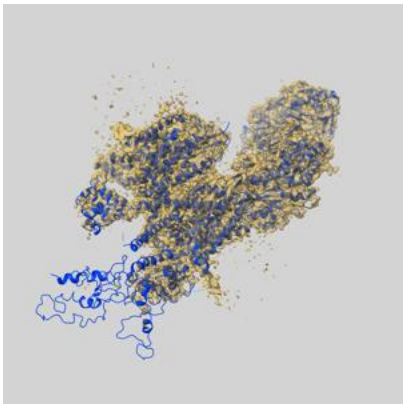
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37475 and PDB model 8WE9. Per-residue inclusion information can be found in section 3 on page 8.

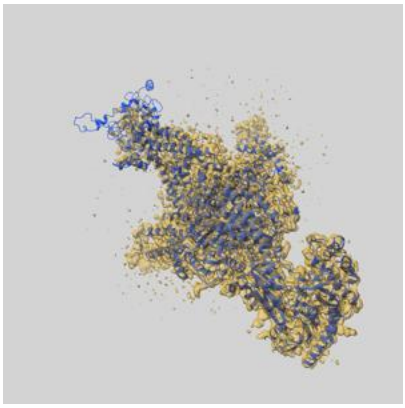
9.1 Map-model overlay



X



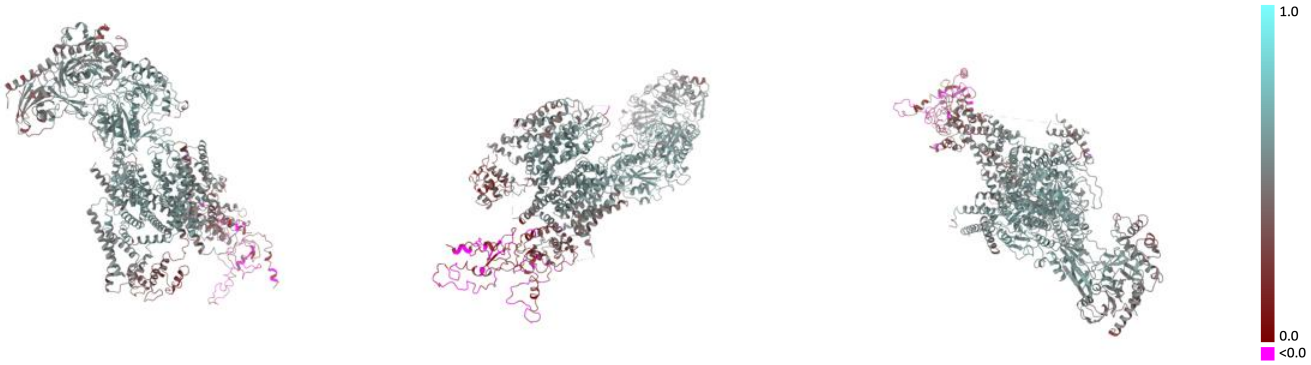
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

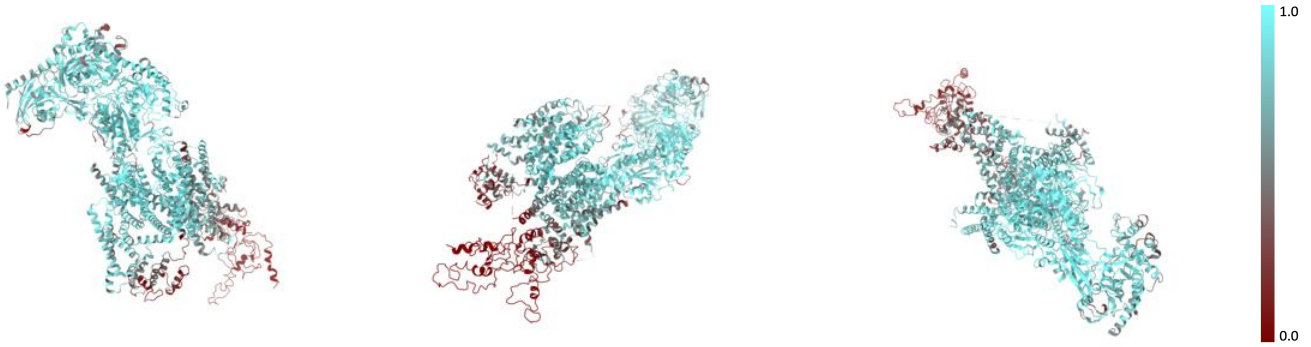
9.2 Q-score mapped to coordinate model (i)



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.

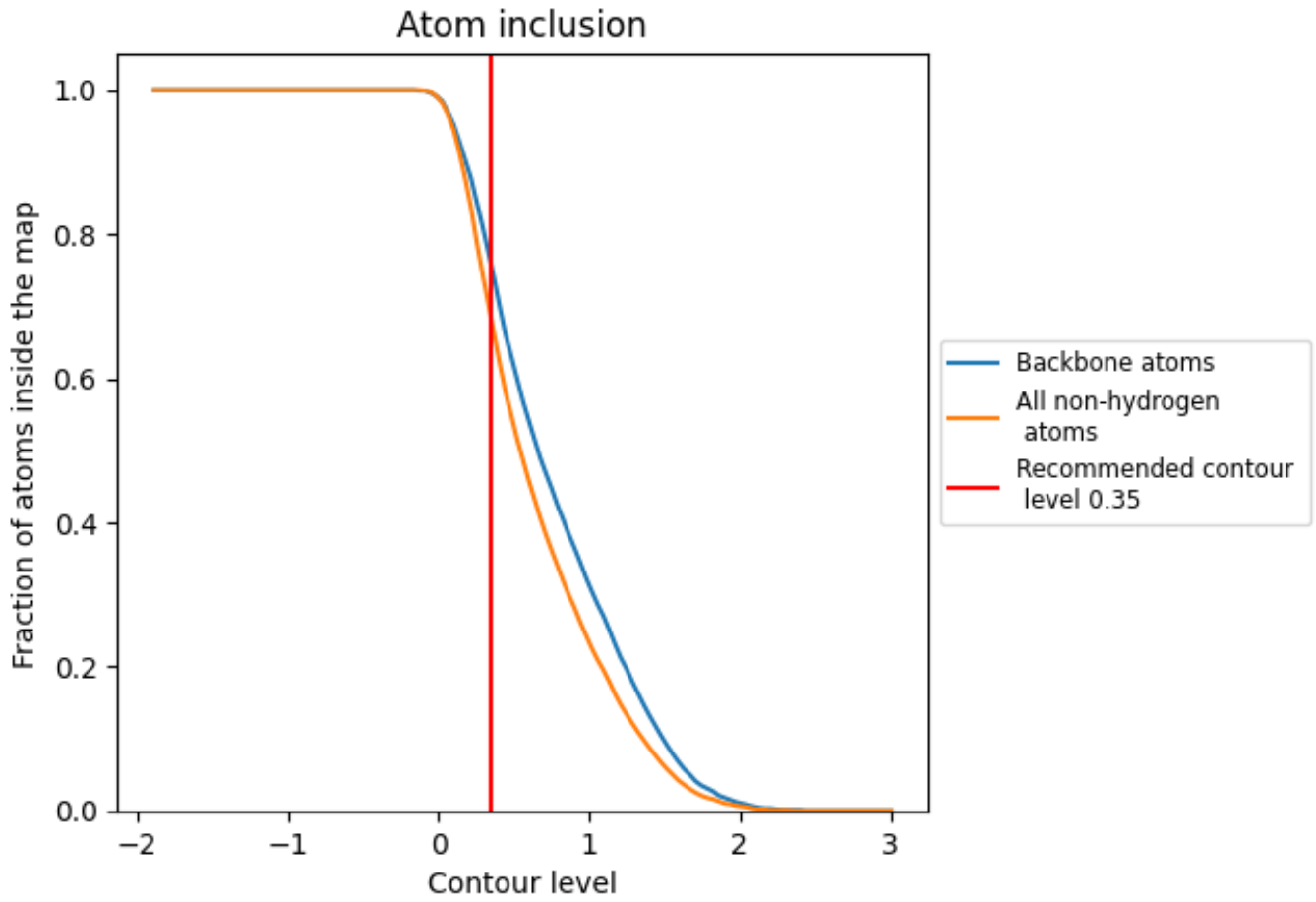
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 68% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6820	0.4700
A	0.7210	0.5040
B	0.5240	0.3740
C	0.0980	0.1590
D	0.8300	0.5300
E	0.2860	0.2910
F	0.6790	0.4340
G	0.4290	0.3510
H	0.6430	0.4270