Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 04:59 AM EST

PDB ID	:	7MIX
EMDB ID	:	EMD-23867
Title	:	Human N-type voltage-gated calcium channel Cav2.2 in the presence of ziconotide at 3.0 Angstrom resolution
Authors	:	Yan, N.; Gao, S.; Yao, X.
Deposited on	:	2021-04-18
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:

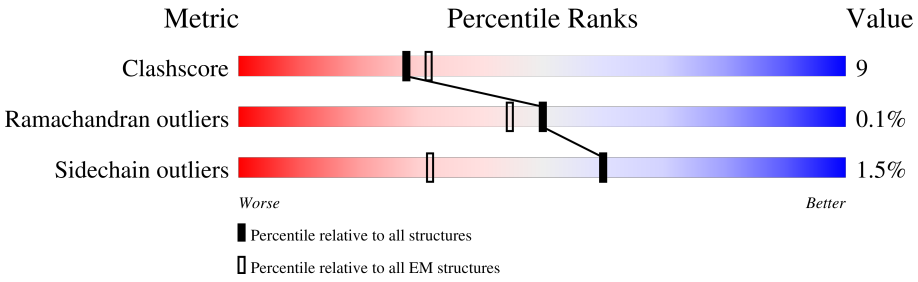
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	2339	10% 45% 11% • 43%
2	B	25	80% 16% •
3	D	1103	7% 68% 18% 14%
4	C	484	44% 50% 17% 33%
5	G	3	33% 33% 33% 33%
6	J	2	100% 100%
6	P	2	50% 100%
6	S	2	50% 50% 50%

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Mol	Chain	Length	Quality of chain
7	L	4	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 21652 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 N-type calcium channel subunit alpha-1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1326	10740	7049	1746	1868	77	1	0

- Molecule 2 is a protein called Omega-conotoxin MVIIA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	25	176	102	35	32	7	0	0

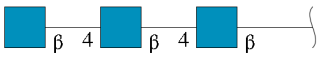
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

- Molecule 4 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

- Molecule 5 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		
5	G	3	42	24	3	15	0	0

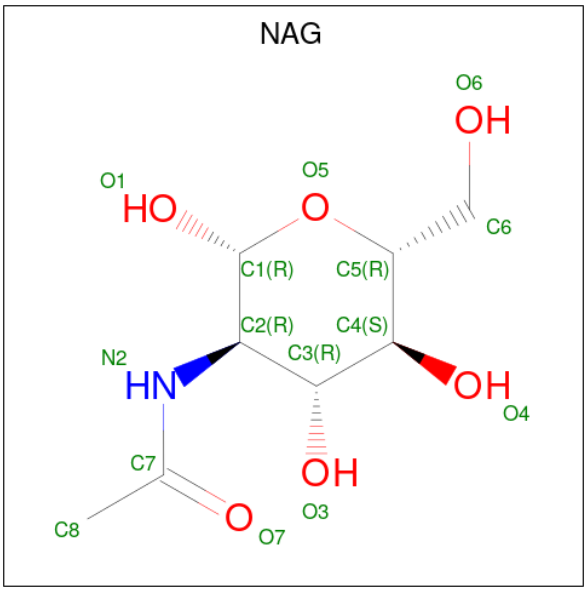
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	L	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

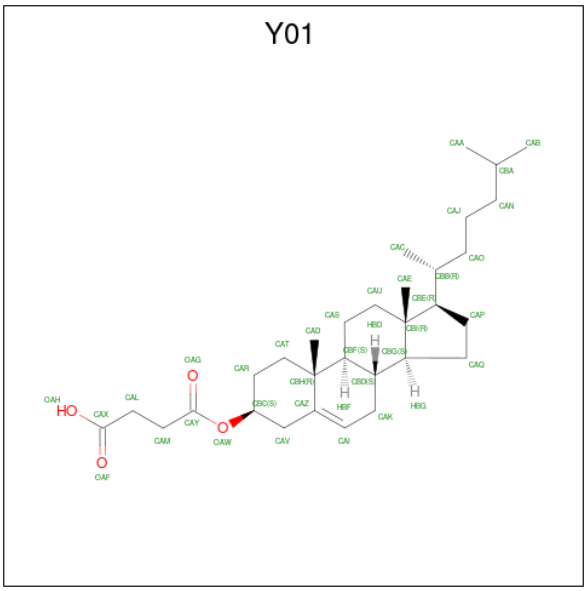


Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 14 8 1 5	0
8	D	1	Total C N O 14 8 1 5	0
8	D	1	Total C N O 14 8 1 5	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

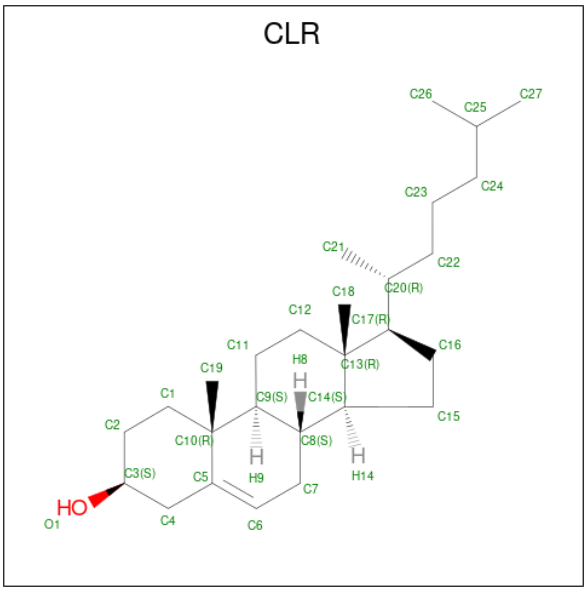
Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total Ca 1 1	0
9	D	1	Total Ca 1 1	0

- Molecule 10 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



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

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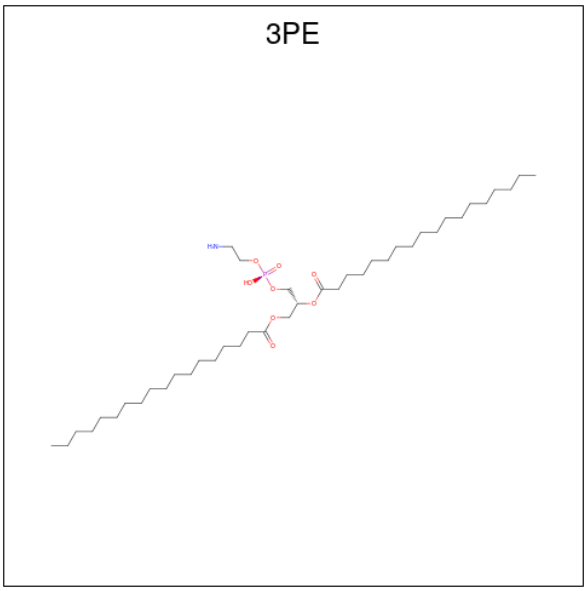
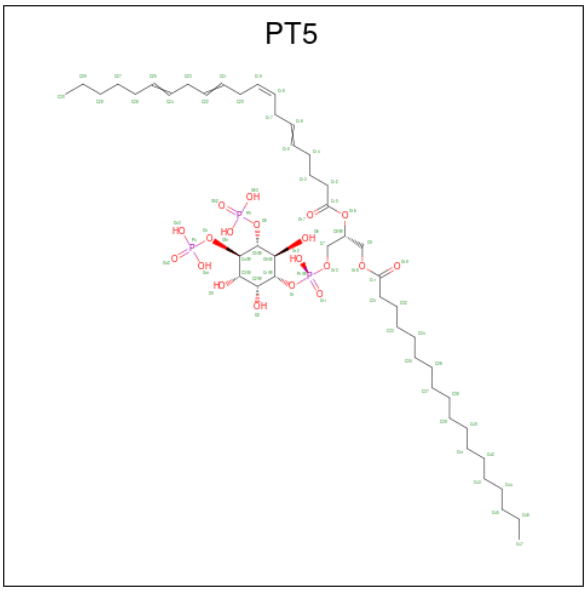
Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C O 28 27 1	0
11	A	1	Total C O 28 27 1	0
11	A	1	Total C O 28 27 1	0
11	A	1	Total C O 28 27 1	0

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C N O P 40 30 1 8 1	0
12	A	1	Total C N O P 51 41 1 8 1	0

- Molecule 13 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: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



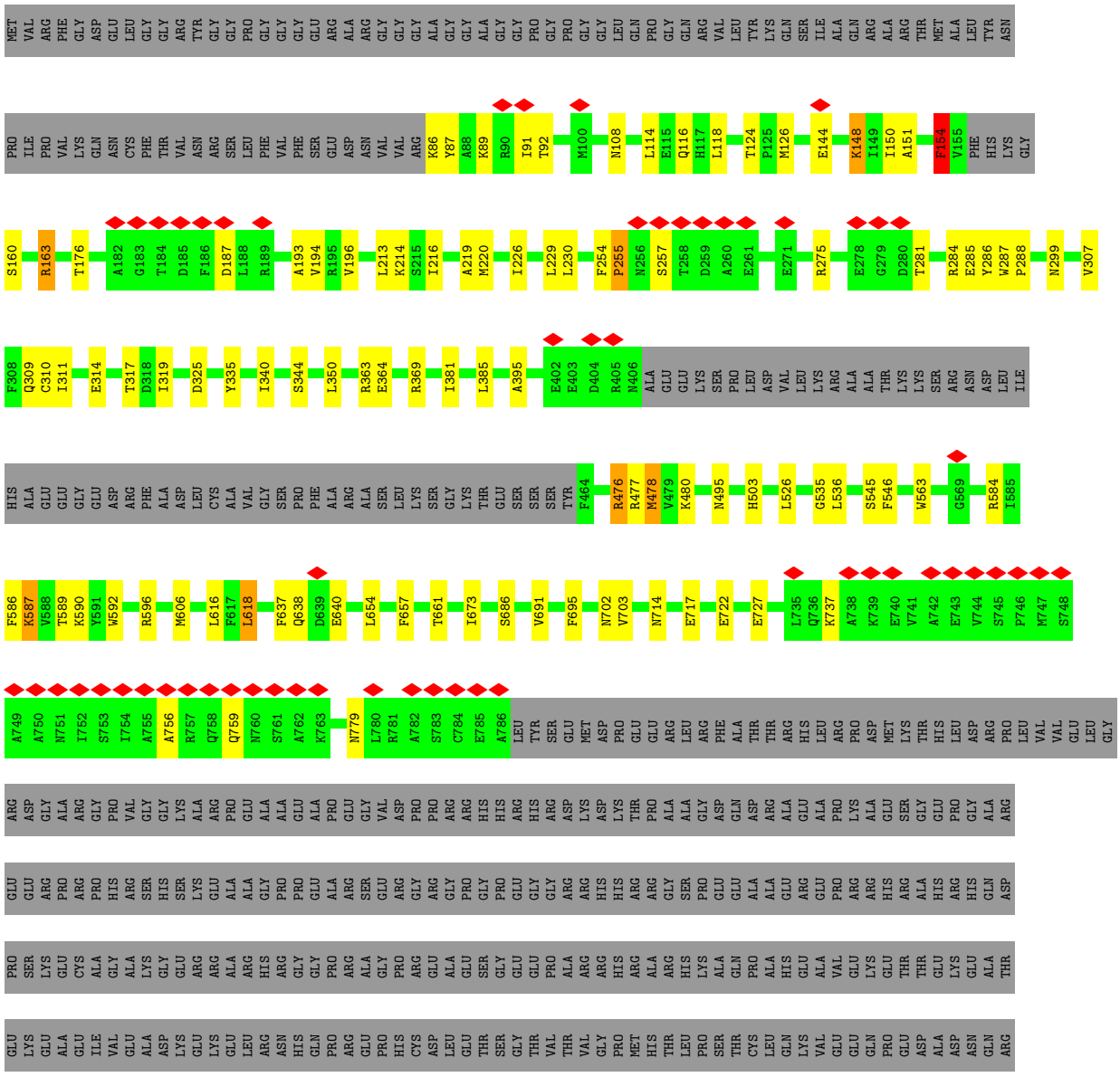
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			64	42	19	3	

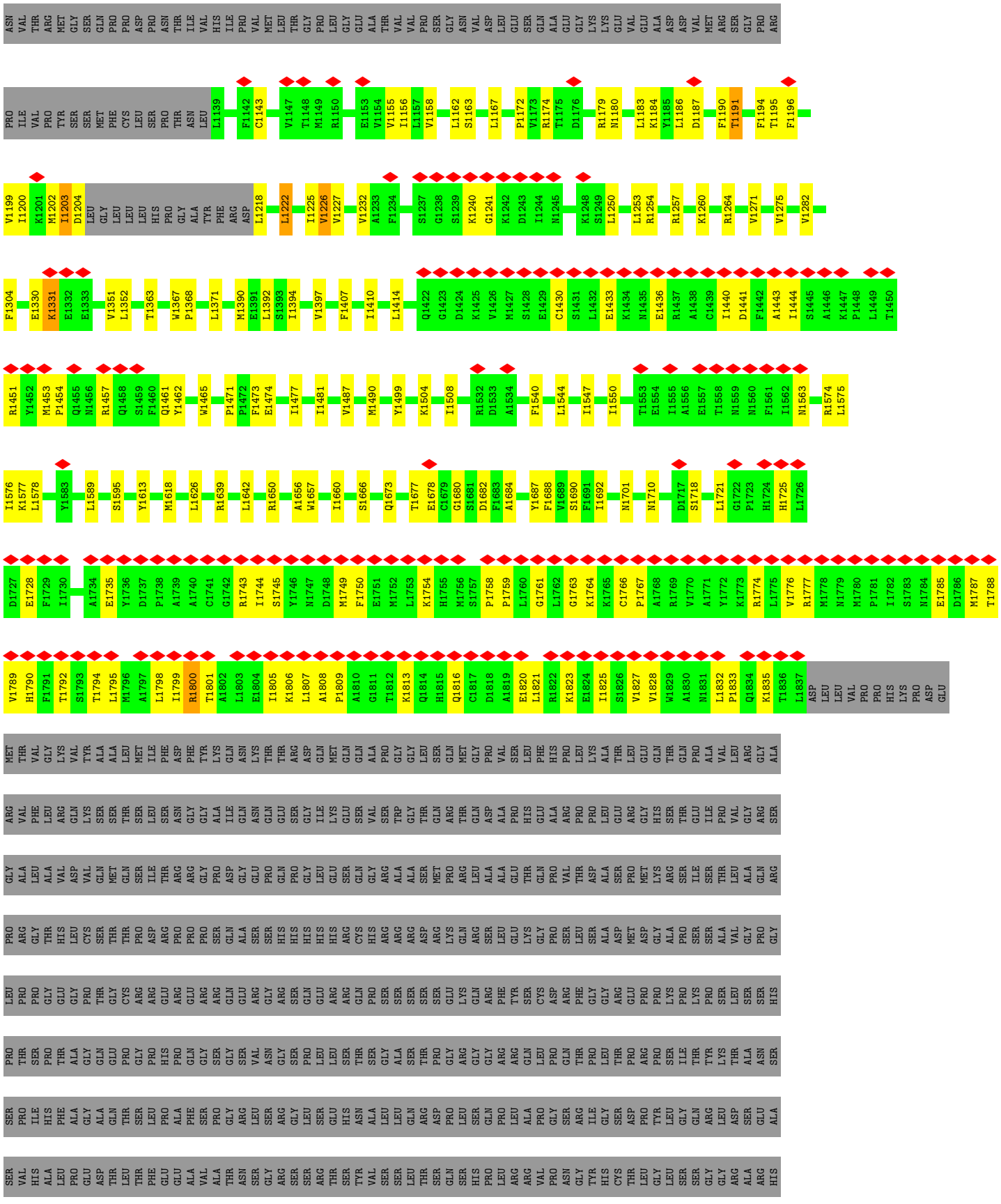
3 Residue-property plots (i)

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 N-type calcium channel subunit alpha-1B

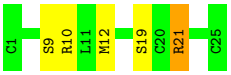
Chain A:





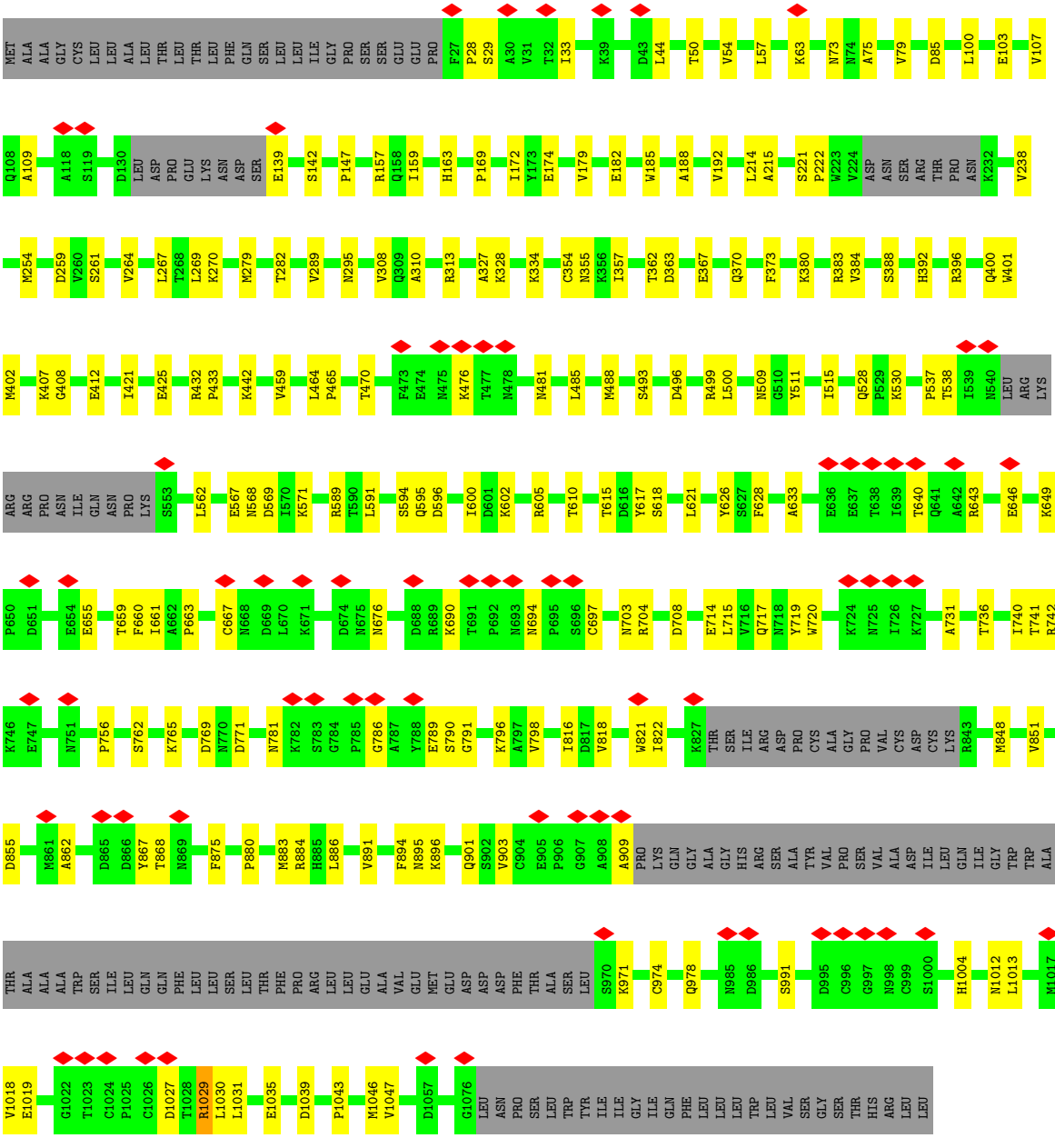
• Molecule 2: Omega-conotoxin MVIIA

Chain B:



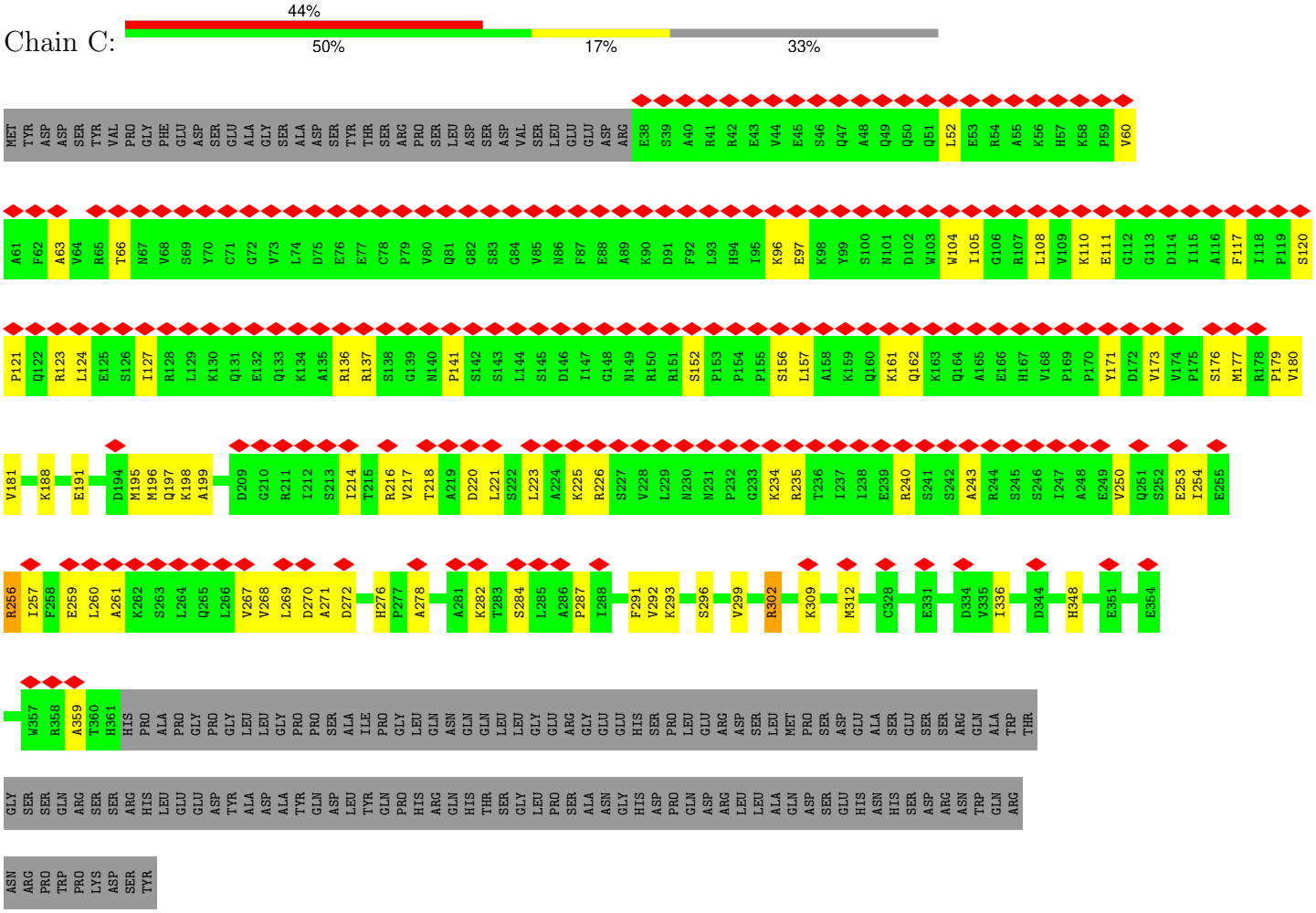
• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:



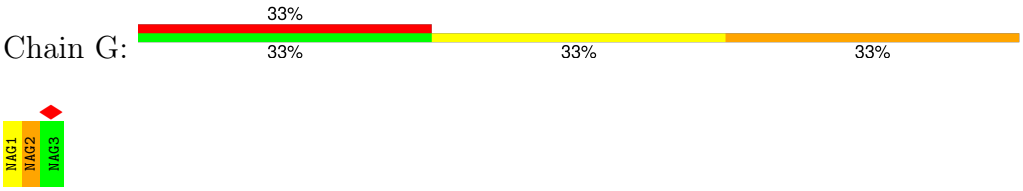
• Molecule 4: Voltage-dependent L-type calcium channel subunit beta-3

Chain C:



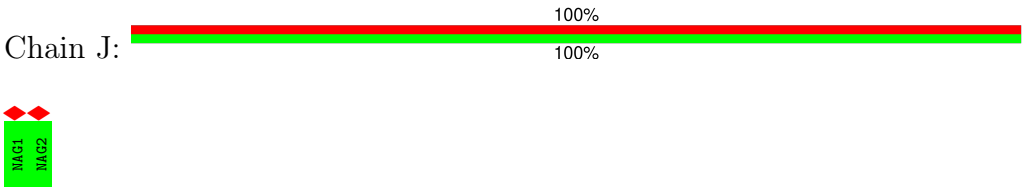
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



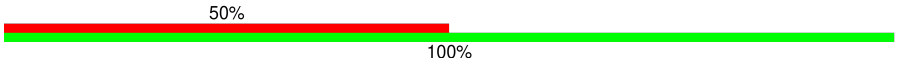
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 7: 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 L:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170839	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	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: CLR, 3PE, Y01, PT5, NAG, CA

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	0.27	0/11002	0.48	2/14897 (0.0%)
2	B	0.26	0/176	0.50	0/228
3	D	0.25	0/7728	0.49	0/10477
4	C	0.25	0/2624	0.51	0/3544
All	All	0.26	0/21530	0.48	2/29146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	596[A]	ARG	CA-C-O	5.86	132.40	120.10
1	A	596[B]	ARG	CA-C-O	5.86	132.40	120.10

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	10740	0	10851	212	0
2	B	176	0	176	5	0
3	D	7570	0	7369	118	0
4	C	2575	0	2619	54	0
5	G	42	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	28	0	25	0	0
6	P	28	0	25	0	0
6	S	28	0	25	1	0
7	L	56	0	49	4	0
8	A	14	0	13	0	0
8	D	28	0	26	1	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	A	70	0	98	16	0
11	A	140	0	230	11	0
12	A	91	0	139	5	0
13	A	64	0	67	12	0
All	All	21652	0	21749	410	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 9.

All (410) 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:1187:ASP:O	1:A:1191:THR:HG22	1.67	0.94
1:A:1195:THR:HG22	1:A:1227:VAL:HG13	1.48	0.94
1:A:254:PHE:HB3	1:A:284:ARG:NH2	1.83	0.92
1:A:160:SER:HA	1:A:163:ARG:HG3	1.52	0.90
1:A:476:ARG:HH11	1:A:476:ARG:HB3	1.35	0.89
1:A:1508:ILE:HG12	1:A:1550:ILE:HD11	1.57	0.87
1:A:476:ARG:HH11	1:A:476:ARG:CB	1.88	0.86
1:A:476:ARG:NH1	1:A:476:ARG:O	2.08	0.86
1:A:1195:THR:HG22	1:A:1227:VAL:CG1	2.09	0.83
10:A:2406:Y01:HAD3	10:A:2406:Y01:CAK	2.10	0.81
1:A:476:ARG:HG3	1:A:535:GLY:O	1.80	0.80
1:A:1397:VAL:HG21	10:A:2403:Y01:HAQ1	1.64	0.78
1:A:546:PHE:CE2	13:A:2412:PT5:H52	2.19	0.76
3:D:660:PHE:HB2	3:D:741:THR:HG22	1.68	0.75
1:A:1186:LEU:O	1:A:1190:PHE:CD2	2.40	0.74
1:A:309:GLN:NE2	1:A:314:GLU:O	2.21	0.73
1:A:1800:ARG:HH12	1:A:1805:ILE:HA	1.52	0.73
13:A:2412:PT5:O12	13:A:2412:PT5:O6	2.05	0.73
1:A:1457:ARG:HA	1:A:1462:TYR:HB2	1.70	0.73
1:A:476:ARG:HG3	1:A:535:GLY:C	2.09	0.72
13:A:2412:PT5:O42	13:A:2412:PT5:O3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:O	1:A:311:ILE:HG23	1.90	0.71
1:A:477:ARG:O	1:A:477:ARG:HG2	1.91	0.70
1:A:1394:ILE:HG13	10:A:2403:Y01:HAD2	1.73	0.69
3:D:85:ASP:HB3	3:D:500:LEU:HD22	1.75	0.69
1:A:86:LYS:HG3	1:A:87:TYR:H	1.58	0.69
4:C:226:ARG:HD2	4:C:284:SER:HB2	1.75	0.68
10:A:2403:Y01:HAU2	10:A:2403:Y01:HAC1	1.74	0.68
1:A:1574:ARG:O	1:A:1577:LYS:HB2	1.94	0.68
1:A:1226:VAL:HG11	1:A:1260:LYS:NZ	2.09	0.67
1:A:335:TYR:HB2	12:A:2411:3PE:H351	1.76	0.66
1:A:229:LEU:HD21	1:A:1589:LEU:HD13	1.77	0.65
3:D:109:ALA:HA	3:D:470:THR:HG22	1.78	0.65
1:A:1186:LEU:O	1:A:1190:PHE:HD2	1.77	0.65
1:A:1642:LEU:HD12	12:A:2410:3PE:H322	1.78	0.65
1:A:1394:ILE:CG1	10:A:2403:Y01:HAD2	2.27	0.65
1:A:1222:LEU:O	1:A:1222:LEU:HD12	1.95	0.65
3:D:731:ALA:HA	3:D:745:PRO:HG2	1.78	0.65
1:A:1444:ILE:HG12	1:A:1832:LEU:HD21	1.78	0.64
4:C:191:GLU:O	4:C:195:MET:HG3	1.97	0.64
1:A:1282:VAL:HG23	1:A:1414:LEU:HD23	1.77	0.64
4:C:216:ARG:HE	4:C:218:THR:HG22	1.61	0.64
4:C:157:LEU:HD23	4:C:162:GLN:HG3	1.80	0.64
1:A:1254:ARG:HG2	1:A:1257:ARG:HE	1.63	0.64
1:A:285:GLU:HA	1:A:285:GLU:OE1	1.97	0.63
4:C:302:ARG:NH1	4:C:302:ARG:HG3	2.12	0.63
1:A:317:THR:HG21	1:A:1650:ARG:HG3	1.79	0.63
1:A:1444:ILE:HG23	1:A:1832:LEU:HD11	1.79	0.63
1:A:254:PHE:CB	1:A:284:ARG:NH2	2.61	0.63
4:C:217:VAL:HB	4:C:271:ALA:HB2	1.80	0.62
3:D:308:VAL:HG12	3:D:1047:VAL:HG21	1.81	0.62
4:C:276:HIS:HD2	4:C:278:ALA:H	1.48	0.62
4:C:292:VAL:O	4:C:292:VAL:HG23	2.00	0.61
3:D:528:GLN:O	3:D:901:GLN:NE2	2.33	0.61
3:D:169:PRO:HG2	3:D:172:ILE:HD12	1.82	0.61
4:C:214:ILE:HG22	4:C:268:VAL:HB	1.81	0.61
1:A:150:ILE:HD12	1:A:150:ILE:O	2.00	0.61
1:A:1776:VAL:HG12	1:A:1777:ARG:H	1.66	0.61
4:C:60:VAL:HA	4:C:96:LYS:HG2	1.82	0.61
1:A:1172:PRO:HG3	1:A:1618:MET:HG2	1.83	0.61
4:C:302:ARG:HH11	4:C:302:ARG:CG	2.14	0.60
1:A:1195:THR:CG2	1:A:1227:VAL:HG13	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:ILE:HG23	1:A:1203:ILE:O	2.01	0.60
1:A:310:CYS:SG	1:A:319:ILE:HD12	2.41	0.60
3:D:855:ASP:HB2	3:D:1012:ASN:HB2	1.82	0.60
3:D:894:PHE:HE2	3:D:896:LYS:HE3	1.66	0.60
1:A:1179:ARG:HB2	11:A:2408:CLR:H191	1.82	0.60
4:C:121:PRO:HD3	4:C:171:TYR:HD2	1.65	0.60
1:A:220:MET:SD	1:A:702:ASN:ND2	2.75	0.60
1:A:1394:ILE:HG13	10:A:2403:Y01:CAD	2.30	0.60
10:A:2406:Y01:HAD3	10:A:2406:Y01:HAK1	1.83	0.59
1:A:1800:ARG:HE	1:A:1807:LEU:HD12	1.66	0.59
3:D:568:ASN:HB3	3:D:571:LYS:HG2	1.83	0.59
3:D:708:ASP:HB3	3:D:736:THR:HG21	1.84	0.59
4:C:181:VAL:HG12	4:C:269:LEU:HB2	1.84	0.59
1:A:476:ARG:HH11	1:A:476:ARG:CG	2.14	0.59
1:A:1650:ARG:HH11	1:A:1660:ILE:HD11	1.67	0.59
2:B:10:ARG:HH12	2:B:19:SER:HB2	1.68	0.59
3:D:594:SER:OG	3:D:596:ASP:O	2.20	0.59
3:D:509:ASN:ND2	3:D:626:TYR:OH	2.36	0.59
4:C:240:ARG:H	4:C:243:ALA:HB3	1.68	0.59
7:L:4:NAG:H83	7:L:4:NAG:H3	1.85	0.58
1:A:545:SER:OG	13:A:2412:PT5:H16	2.03	0.58
1:A:1143:CYS:SG	1:A:1203:ILE:HG21	2.43	0.58
1:A:1222:LEU:HD12	1:A:1222:LEU:C	2.24	0.58
1:A:1790:HIS:O	1:A:1794:THR:N	2.34	0.58
4:C:302:ARG:HG3	4:C:302:ARG:HH11	1.67	0.58
1:A:1626:LEU:HB2	1:A:1639:ARG:HH21	1.68	0.58
1:A:1725:HIS:HD2	1:A:1728:GLU:HB2	1.67	0.58
3:D:54:VAL:HG13	3:D:798:VAL:HG12	1.85	0.58
5:G:2:NAG:H83	5:G:2:NAG:H3	1.85	0.58
1:A:616:LEU:HD12	1:A:703:VAL:HG11	1.85	0.58
1:A:1800:ARG:HH22	1:A:1806:LYS:H	1.51	0.58
1:A:654:LEU:HD13	10:A:2403:Y01:HAK1	1.85	0.57
3:D:661:ILE:HD12	3:D:740:ILE:HG22	1.86	0.57
1:A:144:GLU:O	1:A:148:LYS:HG3	2.04	0.57
3:D:182:GLU:OE1	3:D:185:TRP:NE1	2.32	0.57
3:D:528:GLN:OE1	3:D:530:LYS:NZ	2.36	0.57
4:C:136:ARG:O	4:C:137:ARG:NH1	2.37	0.57
1:A:395:ALA:HB2	4:C:199:ALA:HB2	1.85	0.57
4:C:250:VAL:O	4:C:254:ILE:HG12	2.05	0.57
1:A:546:PHE:CD2	13:A:2412:PT5:H52	2.39	0.56
1:A:1613:TYR:HH	1:A:1690:SER:HG	1.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:GLU:O	1:A:1788:THR:OG1	2.23	0.56
3:D:848:MET:HG2	3:D:1019:GLU:HA	1.85	0.56
4:C:121:PRO:HD3	4:C:171:TYR:CD2	2.40	0.56
1:A:287:TRP:CD1	1:A:288:PRO:HD2	2.40	0.56
1:A:1776:VAL:HB	1:A:1777:ARG:HD2	1.86	0.56
3:D:538:THR:HB	3:D:909:ALA:HB2	1.88	0.56
1:A:1718:SER:HB2	1:A:1721:LEU:HD23	1.88	0.56
1:A:1790:HIS:HB3	1:A:1794:THR:HG23	1.88	0.55
1:A:1218:LEU:HD23	1:A:1218:LEU:O	2.05	0.55
4:C:188:LYS:HD3	4:C:272:ASP:HA	1.88	0.55
1:A:1407:PHE:HA	1:A:1410:ILE:HG12	1.88	0.55
3:D:259:ASP:HB2	3:D:362:THR:HG22	1.88	0.55
3:D:646:GLU:HG3	3:D:649:LYS:HE2	1.88	0.55
1:A:369:ARG:NH1	1:A:717:GLU:OE2	2.40	0.55
1:A:1194:PHE:HE2	1:A:1257:ARG:NH1	2.05	0.55
7:L:3:NAG:H3	7:L:3:NAG:H83	1.89	0.55
13:A:2412:PT5:H55	13:A:2412:PT5:O19	2.05	0.55
2:B:21:ARG:HG3	2:B:21:ARG:HH11	1.72	0.54
3:D:63:LYS:NZ	3:D:714:GLU:OE2	2.27	0.54
3:D:589:ARG:HH12	3:D:602:LYS:HD2	1.73	0.54
4:C:108:LEU:HB3	4:C:110:LYS:HG2	1.89	0.54
1:A:1749:MET:SD	1:A:1790:HIS:ND1	2.81	0.54
1:A:1750:PHE:O	1:A:1754:LYS:NZ	2.40	0.54
1:A:503:HIS:CD2	10:A:2406:Y01:HAR1	2.42	0.54
1:A:586:PHE:O	1:A:589:THR:OG1	2.25	0.54
1:A:1194:PHE:HE2	1:A:1257:ARG:HH11	1.55	0.54
1:A:1744:ILE:HG22	1:A:1745:SER:H	1.72	0.54
1:A:1677:THR:HG23	1:A:1678:GLU:HG3	1.90	0.54
1:A:1745:SER:HA	1:A:1787:MET:HB3	1.89	0.53
3:D:659:THR:OG1	3:D:742:ARG:NH1	2.37	0.53
4:C:104:TRP:HE1	4:C:120:SER:HA	1.73	0.53
4:C:220:ASP:OD1	4:C:221:LEU:N	2.42	0.53
1:A:616:LEU:HD11	1:A:703:VAL:HG21	1.90	0.53
3:D:73:ASN:N	3:D:628:PHE:O	2.40	0.53
1:A:364:GLU:O	1:A:779:ASN:ND2	2.42	0.52
1:A:756:ALA:HA	1:A:759:GLN:HE22	1.74	0.52
3:D:357:ILE:HG22	3:D:383:ARG:HB2	1.92	0.52
1:A:616:LEU:CD1	1:A:703:VAL:HG11	2.40	0.52
3:D:182:GLU:HA	3:D:185:TRP:CD1	2.44	0.52
2:B:10:ARG:NH1	2:B:19:SER:HB2	2.25	0.52
3:D:392:HIS:CE1	3:D:396:ARG:HE	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:CA	1:A:163:ARG:HG3	2.34	0.52
1:A:1504:LYS:O	1:A:1508:ILE:HG13	2.09	0.52
1:A:480:LYS:HZ1	1:A:536:LEU:HD22	1.76	0.51
1:A:584:ARG:HD3	1:A:587:LYS:HZ1	1.74	0.51
1:A:381:ILE:HG23	4:C:299:VAL:HG22	1.92	0.51
1:A:1650:ARG:HH12	1:A:1656:ALA:HB3	1.74	0.51
1:A:1254:ARG:HD2	1:A:1257:ARG:HH21	1.75	0.51
1:A:89:LYS:CD	1:A:151:ALA:HB1	2.39	0.51
1:A:1813:LYS:HE3	1:A:1816:GLN:HB2	1.91	0.51
3:D:515:ILE:HG22	3:D:618:SER:HB2	1.92	0.51
1:A:1218:LEU:HD23	1:A:1218:LEU:C	2.31	0.51
3:D:884:ARG:HH22	3:D:1029:ARG:HG2	1.75	0.51
1:A:476:ARG:NH1	1:A:476:ARG:CG	2.73	0.51
1:A:478:MET:O	1:A:478:MET:HG3	2.10	0.51
1:A:1595:SER:OG	1:A:1710:ASN:ND2	2.33	0.51
3:D:103:GLU:HG2	3:D:192:VAL:HG21	1.93	0.51
1:A:1454:PRO:HB3	1:A:1461:GLN:HE22	1.76	0.51
1:A:340:ILE:O	1:A:344:SER:HB2	2.11	0.51
1:A:616:LEU:CD1	1:A:703:VAL:HG21	2.41	0.51
4:C:123:ARG:HH22	4:C:127:ILE:HD13	1.76	0.51
1:A:255:PRO:HA	1:A:281:THR:HG22	1.93	0.50
1:A:1473:PHE:O	1:A:1477:ILE:HG12	2.11	0.50
1:A:1821:LEU:O	1:A:1825:ILE:HG12	2.11	0.50
3:D:485:LEU:HD22	7:L:1:NAG:H82	1.93	0.50
1:A:1743:ARG:HA	1:A:1789:VAL:HG13	1.92	0.50
3:D:1027:ASP:OD1	3:D:1027:ASP:N	2.45	0.50
3:D:279:MET:O	3:D:282:THR:OG1	2.28	0.50
1:A:1367:TRP:CD1	1:A:1368:PRO:HD3	2.47	0.50
3:D:568:ASN:OD1	3:D:569:ASP:N	2.45	0.50
4:C:156:SER:HB2	4:C:161:LYS:HD3	1.94	0.50
3:D:363:ASP:O	3:D:388:SER:OG	2.28	0.49
4:C:177:MET:H	4:C:261:ALA:HB1	1.77	0.49
2:B:9:SER:HB3	2:B:12:MET:HG2	1.94	0.49
3:D:44:LEU:HD11	3:D:821:TRP:HE1	1.77	0.49
3:D:640:THR:HA	3:D:643:ARG:HG2	1.94	0.49
1:A:1240:LYS:HG2	1:A:1241:GLY:H	1.78	0.49
4:C:104:TRP:HE1	4:C:121:PRO:HD2	1.77	0.49
4:C:216:ARG:HA	4:C:270:ASP:HB2	1.93	0.49
1:A:673:ILE:HD11	1:A:686:SER:HB3	1.94	0.49
1:A:226:ILE:HD12	1:A:350:LEU:HB3	1.95	0.49
3:D:79:VAL:HG12	3:D:610:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:O	1:A:160:SER:N	2.47	0.48
1:A:1684:ALA:HA	1:A:1687:TYR:HB3	1.95	0.48
3:D:676:ASN:ND2	3:D:756:PRO:HB3	2.28	0.48
3:D:880:PRO:HG3	3:D:1030:LEU:HA	1.94	0.48
1:A:691:VAL:HG13	1:A:695:PHE:HD2	1.78	0.48
3:D:1043:PRO:HA	3:D:1046:MET:HB3	1.95	0.48
4:C:309:LYS:HA	4:C:312:MET:HB2	1.95	0.48
1:A:1363:THR:HG21	1:A:1657:TRP:HE1	1.79	0.48
3:D:704:ARG:NH1	3:D:708:ASP:OD2	2.46	0.48
5:G:1:NAG:H61	5:G:2:NAG:H82	1.96	0.48
1:A:89:LYS:HD2	1:A:151:ALA:HB1	1.96	0.48
1:A:587:LYS:HB2	1:A:587:LYS:HE3	1.31	0.48
1:A:1576:ILE:HD12	1:A:1576:ILE:H	1.79	0.48
1:A:1490:MET:HG2	1:A:1499:TYR:OH	2.14	0.47
11:A:2408:CLR:H272	11:A:2408:CLR:H232	1.71	0.47
3:D:851:VAL:HG12	3:D:862:ALA:HA	1.94	0.47
4:C:111:GLU:HA	4:C:359:ALA:HA	1.95	0.47
1:A:727:GLU:HG2	1:A:759:GLN:HG3	1.96	0.47
4:C:141:PRO:HG3	4:C:152:SER:HB3	1.96	0.47
1:A:1186:LEU:HB3	1:A:1190:PHE:CE2	2.49	0.47
3:D:1039:ASP:N	3:D:1039:ASP:OD1	2.46	0.47
4:C:66:THR:HG22	4:C:171:TYR:CE1	2.49	0.47
1:A:1143:CYS:SG	1:A:1203:ILE:CG2	3.02	0.47
1:A:1186:LEU:HB3	1:A:1190:PHE:HE2	1.79	0.47
1:A:144:GLU:O	1:A:148:LYS:CG	2.62	0.47
1:A:1194:PHE:CE2	1:A:1257:ARG:NH1	2.82	0.47
13:A:2412:PT5:HO3	13:A:2412:PT5:P4	2.33	0.47
1:A:1832:LEU:O	1:A:1835:LYS:N	2.48	0.47
1:A:637:PHE:CD1	1:A:638:GLN:HG3	2.50	0.47
3:D:690:LYS:HZ1	3:D:694:ASN:HA	1.80	0.47
4:C:234:LYS:HG3	4:C:235:ARG:HG2	1.97	0.47
1:A:114:LEU:HD13	1:A:126:MET:CE	2.45	0.46
1:A:363:ARG:NH2	1:A:717:GLU:OE1	2.41	0.46
1:A:1451:ARG:HH12	1:A:1735:GLU:HA	1.79	0.46
1:A:118:LEU:HD11	1:A:124:THR:HG23	1.97	0.46
1:A:480:LYS:NZ	1:A:536:LEU:HD22	2.29	0.46
3:D:895:ASN:OD1	6:S:1:NAG:O3	2.18	0.46
1:A:160:SER:HA	1:A:163:ARG:CG	2.36	0.46
1:A:385:LEU:CD1	4:C:302:ARG:HB3	2.45	0.46
3:D:442:LYS:NZ	3:D:465:PRO:O	2.34	0.46
1:A:91:ILE:HG13	1:A:92:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2406:Y01:HAS2	10:A:2406:Y01:HAE1	1.54	0.46
3:D:781:ASN:OD1	8:D:1202:NAG:H2	2.16	0.46
1:A:640:GLU:HG2	3:D:267:LEU:HD13	1.98	0.46
1:A:1440:ILE:HG12	1:A:1799:ILE:HD12	1.97	0.46
1:A:1471:PRO:O	1:A:1474:GLU:HG3	2.16	0.46
3:D:215:ALA:HB2	3:D:238:VAL:HG21	1.98	0.46
3:D:373:PHE:CE2	3:D:402:MET:HG2	2.51	0.46
4:C:180:VAL:HB	4:C:268:VAL:HG22	1.98	0.46
1:A:1743:ARG:HD3	1:A:1788:THR:HG23	1.98	0.46
3:D:264:VAL:O	3:D:269:LEU:HB2	2.16	0.46
3:D:295:ASN:ND2	3:D:328:LYS:O	2.39	0.46
3:D:459:VAL:HG12	3:D:493:SER:HA	1.97	0.46
1:A:1174:ARG:O	1:A:1180:ASN:ND2	2.49	0.45
3:D:509:ASN:HB3	3:D:605:ARG:HH12	1.81	0.45
4:C:179:PRO:HG2	4:C:287:PRO:HB3	1.98	0.45
1:A:1226:VAL:HG11	1:A:1260:LYS:HZ2	1.78	0.45
1:A:1792:THR:HG22	1:A:1835:LYS:HG2	1.99	0.45
1:A:1832:LEU:N	1:A:1833:PRO:HD2	2.30	0.45
3:D:396:ARG:NH1	3:D:412:GLU:OE2	2.50	0.45
1:A:275:ARG:HB2	1:A:325:ASP:HB2	1.98	0.45
1:A:1776:VAL:HG12	1:A:1777:ARG:N	2.30	0.45
4:C:223:LEU:HA	4:C:225:LYS:HE2	1.97	0.45
4:C:291:PHE:HB3	4:C:336:ILE:HD12	1.97	0.45
1:A:1795:LEU:O	1:A:1799:ILE:HG12	2.17	0.45
1:A:1828:VAL:HG12	1:A:1828:VAL:O	2.17	0.45
3:D:464:LEU:HD12	3:D:465:PRO:HD2	1.98	0.45
1:A:1271:VAL:O	1:A:1275:VAL:HG23	2.17	0.45
12:A:2411:3PE:H3C2	12:A:2411:3PE:H2G2	1.99	0.45
1:A:1441:ASP:HA	1:A:1444:ILE:HB	1.99	0.45
3:D:537:PRO:HD3	3:D:974:CYS:HB3	1.99	0.45
1:A:230:LEU:HD11	1:A:311:ILE:HD12	1.99	0.45
1:A:1774:ARG:HE	1:A:1801:THR:HG21	1.82	0.45
1:A:1196:PHE:O	1:A:1196:PHE:CD1	2.70	0.44
3:D:289:VAL:HG12	3:D:310:ALA:HB2	1.99	0.44
1:A:187:ASP:OD1	1:A:187:ASP:N	2.50	0.44
1:A:213:LEU:HA	1:A:216:ILE:HG22	1.99	0.44
10:A:2403:Y01:HAE1	10:A:2403:Y01:HAS2	1.55	0.44
11:A:2404:CLR:H213	11:A:2404:CLR:H231	1.65	0.44
3:D:267:LEU:HA	3:D:270:LYS:HG2	1.98	0.44
3:D:789:GLU:N	3:D:789:GLU:OE1	2.50	0.44
1:A:363:ARG:HH21	1:A:714:ASN:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:MET:HB2	10:A:2403:Y01:HAM1	2.00	0.44
1:A:1453:MET:HG3	1:A:1465:TRP:CZ2	2.52	0.44
1:A:1761:GLY:HA2	1:A:1798:LEU:HD11	2.00	0.44
4:C:97:GLU:HG2	4:C:105:ILE:HD13	1.99	0.44
1:A:1800:ARG:NH1	1:A:1800:ARG:O	2.50	0.44
2:B:21:ARG:HG3	2:B:21:ARG:NH1	2.33	0.44
3:D:29:SER:O	3:D:33:ILE:HG12	2.16	0.44
3:D:54:VAL:HG21	3:D:796:LYS:HG2	1.99	0.44
1:A:1180:ASN:HA	1:A:1183:LEU:HD12	2.00	0.44
3:D:384:VAL:O	3:D:408:GLY:HA3	2.18	0.44
3:D:791:GLY:HA3	3:D:816:ILE:O	2.16	0.44
1:A:1155:VAL:HA	1:A:1158:VAL:HG12	1.98	0.44
1:A:1163:SER:OG	1:A:1257:ARG:HD3	2.18	0.44
1:A:385:LEU:HD11	4:C:302:ARG:HB3	2.00	0.44
1:A:1180:ASN:O	1:A:1184:LYS:HG3	2.17	0.44
1:A:1575:LEU:O	1:A:1578:LEU:HG	2.17	0.44
11:A:2409:CLR:H272	11:A:2409:CLR:H231	1.79	0.44
4:C:52:LEU:HD11	4:C:117:PHE:HE1	1.83	0.44
3:D:786:GLY:HA2	3:D:790:SER:HB2	2.00	0.44
1:A:1232:VAL:HG12	1:A:1250:LEU:CD1	2.48	0.43
10:A:2403:Y01:HAD3	10:A:2403:Y01:HBD	1.67	0.43
10:A:2406:Y01:HAO1	10:A:2406:Y01:HAP1	1.78	0.43
4:C:124:LEU:HD22	4:C:171:TYR:CZ	2.53	0.43
1:A:1218:LEU:C	1:A:1218:LEU:CD2	2.86	0.43
3:D:157:ARG:NH1	3:D:222:PRO:O	2.50	0.43
3:D:179:VAL:HG23	3:D:214:LEU:HD23	2.00	0.43
3:D:655:GLU:OE1	3:D:717:GLN:NE2	2.49	0.43
4:C:256:ARG:NH1	4:C:260:LEU:HB2	2.32	0.43
1:A:1430:CYS:SG	1:A:1433:GLU:HB2	2.59	0.43
3:D:481:ASN:OD1	7:L:1:NAG:O6	2.32	0.43
1:A:1225:ILE:HG22	1:A:1253:LEU:HD21	2.00	0.43
11:A:2408:CLR:H161	11:A:2408:CLR:H222	1.90	0.43
1:A:176:THR:HG21	1:A:194:VAL:HG21	1.99	0.43
1:A:1162:LEU:HD22	11:A:2408:CLR:H261	1.99	0.43
1:A:1487:VAL:HA	1:A:1490:MET:HE3	2.01	0.43
1:A:257:SER:HA	1:A:284:ARG:NH2	2.33	0.43
1:A:1330:GLU:O	1:A:1331:LYS:HG3	2.18	0.43
1:A:1688:PHE:O	1:A:1692:ILE:HG12	2.18	0.43
13:A:2412:PT5:H39	13:A:2412:PT5:H35	1.67	0.43
3:D:313:ARG:HD2	3:D:313:ARG:HA	1.79	0.43
4:C:179:PRO:HA	4:C:267:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:496:ASP:OD1	3:D:499:ARG:NH1	2.52	0.43
3:D:28:PRO:HB2	3:D:33:ILE:HD11	2.00	0.43
3:D:589:ARG:NH1	3:D:602:LYS:HD2	2.33	0.43
3:D:605:ARG:NH2	3:D:769:ASP:OD1	2.51	0.43
1:A:1394:ILE:HG21	11:A:2404:CLR:H72	2.00	0.43
1:A:1477:ILE:O	1:A:1481:ILE:HG12	2.18	0.43
1:A:1827:VAL:O	1:A:1827:VAL:HG13	2.18	0.43
3:D:421:ILE:O	3:D:425:GLU:HG2	2.19	0.43
1:A:1828:VAL:HG11	1:A:1832:LEU:HD13	2.01	0.43
13:A:2412:PT5:H29	13:A:2412:PT5:H25	1.87	0.43
3:D:100:LEU:HB3	3:D:488:MET:SD	2.59	0.43
3:D:139:GLU:OE2	3:D:142:SER:OG	2.29	0.43
11:A:2404:CLR:H162	11:A:2404:CLR:H221	1.73	0.42
3:D:875:PHE:HB3	3:D:883:MET:SD	2.59	0.42
1:A:476:ARG:HB3	1:A:476:ARG:NH1	2.18	0.42
1:A:1351:VAL:HG13	1:A:1352:LEU:HD12	2.00	0.42
1:A:1682:ASP:HB2	11:A:2409:CLR:H112	2.00	0.42
3:D:254:MET:O	3:D:289:VAL:HA	2.20	0.42
3:D:595:GLN:HB2	3:D:765:LYS:HE3	2.00	0.42
1:A:214:LYS:HB3	1:A:214:LYS:HE2	1.83	0.42
12:A:2411:3PE:H2A2	12:A:2411:3PE:H2D2	1.83	0.42
3:D:991:SER:HB3	3:D:1004:HIS:CD2	2.53	0.42
1:A:657:PHE:O	1:A:661:THR:HG23	2.20	0.42
1:A:1766:CYS:HB3	1:A:1767:PRO:HD3	2.02	0.42
1:A:1304:PHE:CE1	1:A:1392:LEU:HD13	2.55	0.42
3:D:396:ARG:O	3:D:400:GLN:HG3	2.19	0.42
3:D:862:ALA:HB1	3:D:867:TYR:HB2	2.00	0.42
4:C:256:ARG:O	4:C:259:GLU:HG3	2.20	0.42
3:D:591:LEU:HD13	3:D:600:ILE:HG21	2.02	0.42
4:C:257:ILE:HD12	4:C:269:LEU:HD21	2.02	0.42
1:A:476:ARG:NH1	1:A:476:ARG:C	2.73	0.42
1:A:1481:ILE:HG22	1:A:1578:LEU:HD23	2.02	0.42
1:A:1540:PHE:O	1:A:1544:LEU:HD23	2.20	0.42
1:A:546:PHE:CE2	13:A:2412:PT5:C31	2.98	0.42
1:A:737:LYS:HG2	4:C:348:HIS:CE1	2.54	0.42
1:A:1156:ILE:HG21	1:A:1264:ARG:HH21	1.84	0.42
1:A:1820:GLU:HA	1:A:1823:LYS:HG2	2.02	0.42
3:D:978:GLN:NE2	3:D:1035:GLU:OE2	2.34	0.42
4:C:282:LYS:HB2	4:C:282:LYS:HE2	1.85	0.42
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.88	0.41
10:A:2403:Y01:HAP1	10:A:2403:Y01:HAO1	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:159:ILE:HG22	3:D:221:SER:OG	2.20	0.41
3:D:511:TYR:O	3:D:621:LEU:HD12	2.20	0.41
3:D:719:TYR:HD2	3:D:720:TRP:HD1	1.68	0.41
4:C:188:LYS:HE2	4:C:197:GLN:HE22	1.85	0.41
1:A:299:ASN:HD22	11:A:2405:CLR:H12	1.85	0.41
3:D:663:PRO:HD3	3:D:756:PRO:HB2	2.02	0.41
3:D:667:CYS:HB3	3:D:697:CYS:HA	2.02	0.41
1:A:654:LEU:HD21	1:A:1371:LEU:HD21	2.03	0.41
3:D:75:ALA:O	3:D:79:VAL:HG23	2.21	0.41
1:A:592:TRP:CH2	13:A:2412:PT5:O17	2.73	0.41
3:D:57:LEU:HD13	3:D:715:LEU:HD22	2.01	0.41
3:D:185:TRP:HA	5:G:1:NAG:H82	2.03	0.41
1:A:1825:ILE:HD12	1:A:1832:LEU:HD22	2.03	0.41
3:D:174:GLU:HA	3:D:179:VAL:HG11	2.02	0.41
3:D:354:CYS:SG	3:D:355:ASN:N	2.90	0.41
1:A:1666:SER:HA	1:A:1680:GLY:O	2.20	0.41
3:D:107:VAL:HG11	3:D:188:ALA:HB3	2.01	0.41
3:D:595:GLN:HB3	3:D:762:SER:HB2	2.01	0.41
3:D:880:PRO:HB3	3:D:1031:LEU:H	1.84	0.41
3:D:1018:VAL:HG22	3:D:1019:GLU:H	1.85	0.41
1:A:1626:LEU:HD22	1:A:1639:ARG:HE	1.85	0.41
1:A:1813:LYS:HD2	1:A:1813:LYS:HA	1.71	0.41
3:D:50:THR:O	3:D:719:TYR:OH	2.22	0.41
3:D:903:VAL:HG22	3:D:971:LYS:HB3	2.03	0.41
3:D:1018:VAL:HG13	3:D:1019:GLU:O	2.20	0.41
4:C:196:MET:HE3	4:C:196:MET:HB3	1.94	0.41
4:C:253:GLU:O	4:C:257:ILE:HG12	2.21	0.41
1:A:722:GLU:O	1:A:722:GLU:HG2	2.21	0.41
1:A:1763:GLY:O	1:A:1764:LYS:HE2	2.21	0.41
10:A:2403:Y01:HAS1	10:A:2403:Y01:HAT1	1.61	0.41
3:D:261:SER:O	3:D:327:ALA:HB1	2.21	0.41
3:D:334:LYS:NZ	3:D:367:GLU:OE2	2.34	0.41
3:D:380:LYS:HE3	3:D:407:LYS:NZ	2.35	0.41
1:A:1232:VAL:CG1	1:A:1250:LEU:HD11	2.51	0.41
1:A:1547:ILE:HA	1:A:1550:ILE:HG22	2.03	0.41
1:A:1650:ARG:NH1	1:A:1660:ILE:HD11	2.35	0.41
3:D:562:LEU:HD22	3:D:567:GLU:HG3	2.03	0.41
1:A:1808:ALA:HB3	1:A:1809:PRO:HD3	2.02	0.41
3:D:370:GLN:HG3	3:D:401:TRP:CH2	2.56	0.41
3:D:633:ALA:HB3	3:D:703:ASN:HB3	2.02	0.41
3:D:771:ASP:OD1	3:D:771:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:862:ALA:HB3	3:D:868:THR:OG1	2.22	0.41
3:D:886:LEU:O	3:D:891:VAL:HG12	2.20	0.41
1:A:148:LYS:HB3	1:A:148:LYS:HE3	1.63	0.40
1:A:1433:GLU:HG2	1:A:1436:GLU:HB2	2.03	0.40
1:A:1490:MET:HA	11:A:2405:CLR:H212	2.03	0.40
3:D:147:PRO:HB3	3:D:163:HIS:NE2	2.36	0.40
3:D:432:ARG:HB2	3:D:433:PRO:HD3	2.02	0.40
3:D:615:THR:HG23	3:D:617:TYR:H	1.87	0.40
4:C:63:ALA:HB3	4:C:176:SER:HA	2.02	0.40
1:A:193:ALA:O	1:A:196:VAL:HG22	2.22	0.40
1:A:1367:TRP:CG	1:A:1368:PRO:HD3	2.56	0.40
1:A:1563:ASN:ND2	12:A:2411:3PE:H12	2.36	0.40
1:A:1758:PRO:N	1:A:1759:PRO:HD2	2.36	0.40
4:C:173:VAL:H	4:C:226:ARG:HH12	1.68	0.40
1:A:219:ALA:HB3	1:A:702:ASN:HD21	1.86	0.40
1:A:1167:LEU:HD11	1:A:1257:ARG:HD2	2.04	0.40
1:A:1443:ALA:O	1:A:1835:LYS:NZ	2.54	0.40
13:A:2412:PT5:H27	13:A:2412:PT5:H31	1.55	0.40
3:D:818:VAL:O	3:D:822:ILE:HG12	2.22	0.40
3:D:1013:LEU:HD23	3:D:1013:LEU:HA	1.92	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	1317/2339 (56%)	1237 (94%)	77 (6%)	3 (0%)	44 77
2	B	23/25 (92%)	23 (100%)	0	0	100 100
3	D	936/1103 (85%)	895 (96%)	41 (4%)	0	100 100
4	C	322/484 (66%)	307 (95%)	15 (5%)	0	100 100
All	All	2598/3951 (66%)	2462 (95%)	133 (5%)	3 (0%)	50 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	PHE
1	A	286	TYR
1	A	255	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1165/1991 (58%)	1139 (98%)	26 (2%)	47 76
2	B	20/20 (100%)	19 (95%)	1 (5%)	20 53
3	D	837/971 (86%)	835 (100%)	2 (0%)	92 97
4	C	287/426 (67%)	282 (98%)	5 (2%)	56 81
All	All	2309/3408 (68%)	2275 (98%)	34 (2%)	60 83

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	116	GLN
1	A	148	LYS
1	A	154	PHE
1	A	163	ARG
1	A	476	ARG
1	A	478	MET
1	A	495	ASN
1	A	526	LEU
1	A	563	TRP
1	A	587	LYS
1	A	590	LYS
1	A	606	MET
1	A	618	LEU
1	A	1191	THR
1	A	1199	VAL
1	A	1200	ILE

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Mol	Chain	Res	Type
1	A	1202	MET
1	A	1203	ILE
1	A	1204	ASP
1	A	1222	LEU
1	A	1226	VAL
1	A	1331	LYS
1	A	1673	GLN
1	A	1701	ASN
1	A	1800	ARG
2	B	21	ARG
3	D	476	LYS
3	D	1029	ARG
4	C	198	LYS
4	C	256	ARG
4	C	293	LYS
4	C	296	SER
4	C	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	702	ASN
1	A	1673	GLN
1	A	1725	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
5	NAG	G	1	5,3	14,14,15	0.50	0	17,19,21	0.58	0
5	NAG	G	2	5	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
5	NAG	G	3	5	14,14,15	0.35	0	17,19,21	0.38	0
6	NAG	J	1	6,3	14,14,15	0.35	0	17,19,21	0.53	0
6	NAG	J	2	6	14,14,15	0.47	0	17,19,21	0.79	0
7	NAG	L	1	7,3	14,14,15	0.26	0	17,19,21	0.46	0
7	NAG	L	2	7	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	L	3	7	14,14,15	0.97	1 (7%)	17,19,21	1.73	2 (11%)
7	NAG	L	4	7	14,14,15	0.56	0	17,19,21	1.34	2 (11%)
6	NAG	P	1	6,3	14,14,15	0.28	0	17,19,21	0.49	0
6	NAG	P	2	6	14,14,15	0.47	0	17,19,21	0.56	0
6	NAG	S	1	6,3	14,14,15	0.89	2 (14%)	17,19,21	1.26	1 (5%)
6	NAG	S	2	6	14,14,15	0.22	0	17,19,21	0.47	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
5	NAG	G	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	6/6/23/26	0/1/1/1
5	NAG	G	3	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	J	2	6	-	4/6/23/26	0/1/1/1
7	NAG	L	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	NAG	L	3	7	-	6/6/23/26	0/1/1/1
7	NAG	L	4	7	-	6/6/23/26	0/1/1/1
6	NAG	P	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	3	NAG	O5-C1	3.02	1.48	1.43
6	S	1	NAG	O5-C1	2.46	1.47	1.43
6	S	1	NAG	C1-C2	2.15	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	1	NAG	C1-O5-C5	4.87	118.71	112.19
7	L	3	NAG	C1-O5-C5	4.66	118.42	112.19
7	L	3	NAG	C2-N2-C7	4.62	129.09	122.90
7	L	4	NAG	C2-N2-C7	4.56	129.02	122.90
5	G	2	NAG	C2-N2-C7	4.53	128.97	122.90
7	L	4	NAG	C1-C2-N2	2.11	113.76	110.43
5	G	2	NAG	C1-C2-N2	2.07	113.70	110.43

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
7	L	3	NAG	C4-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
7	L	3	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
5	G	3	NAG	C4-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
5	G	3	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
7	L	2	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	G	3	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	G	3	NAG	O7-C7-N2-C2
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
7	L	3	NAG	C8-C7-N2-C2
7	L	3	NAG	O7-C7-N2-C2
7	L	4	NAG	C8-C7-N2-C2
7	L	4	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
7	L	4	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
7	L	4	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	J	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
5	G	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
7	L	3	NAG	C1-C2-N2-C7
7	L	4	NAG	C1-C2-N2-C7
5	G	2	NAG	C3-C2-N2-C7
6	J	2	NAG	C3-C2-N2-C7
7	L	3	NAG	C3-C2-N2-C7
7	L	4	NAG	C3-C2-N2-C7

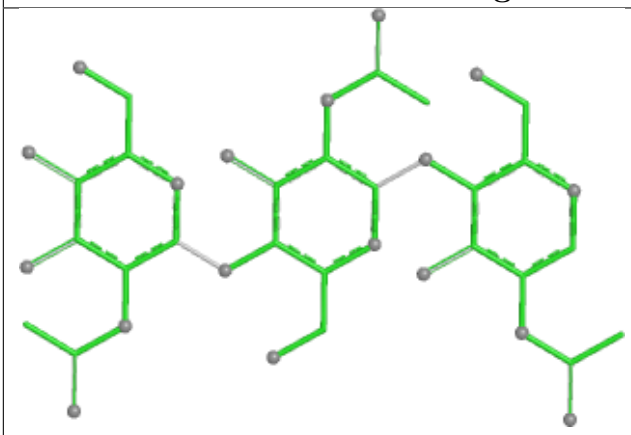
There are no ring outliers.

6 monomers are involved in 8 short contacts:

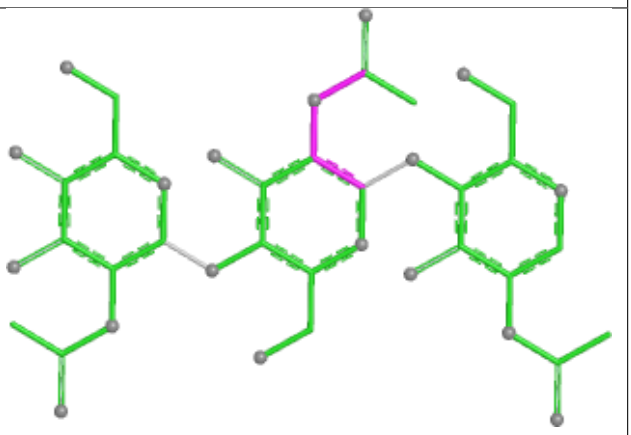
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2	NAG	2	0
7	L	4	NAG	1	0
7	L	1	NAG	2	0
6	S	1	NAG	1	0
7	L	3	NAG	1	0
5	G	1	NAG	2	0

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

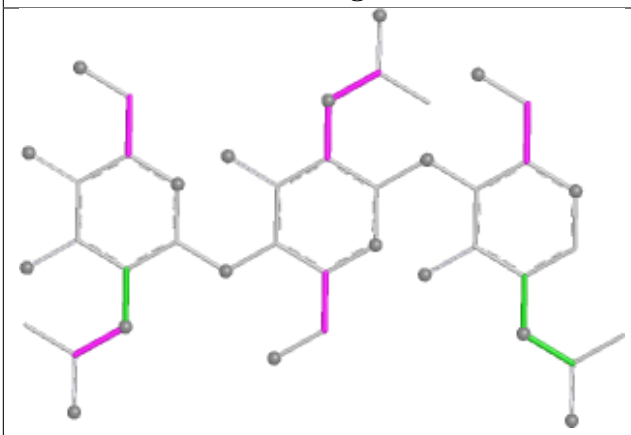
Oligosaccharide Chain G



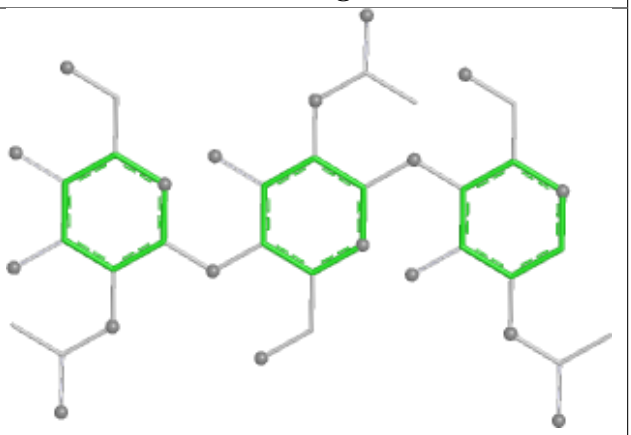
Bond lengths



Bond angles

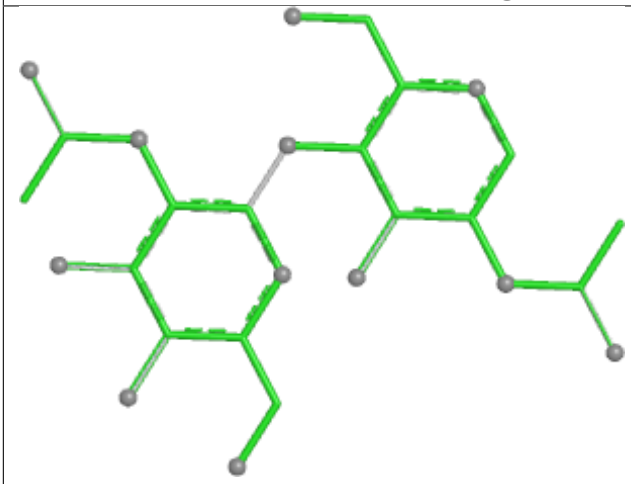


Torsions

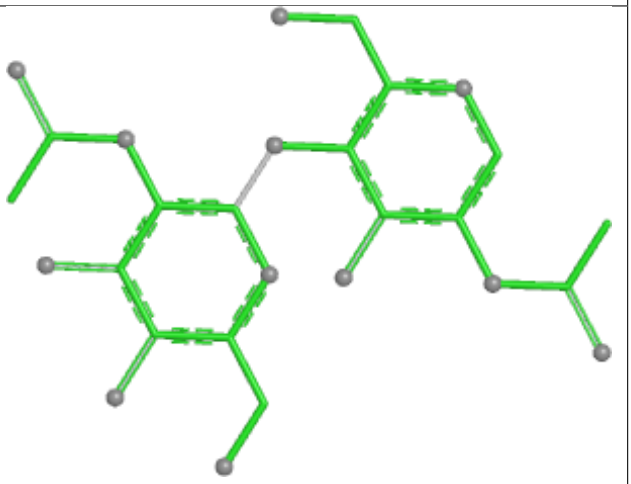


Rings

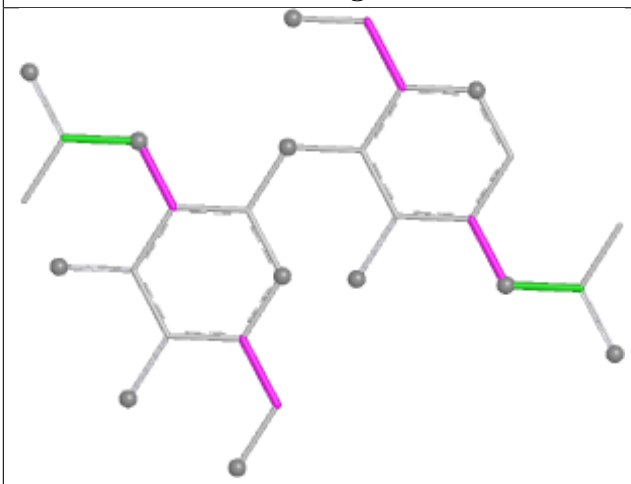
Oligosaccharide Chain J



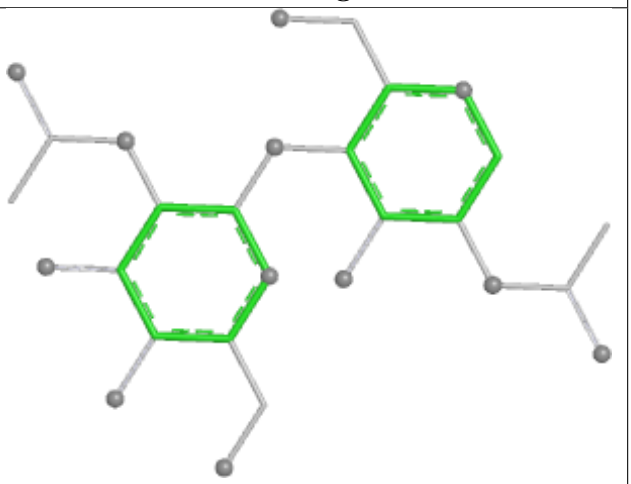
Bond lengths



Bond angles

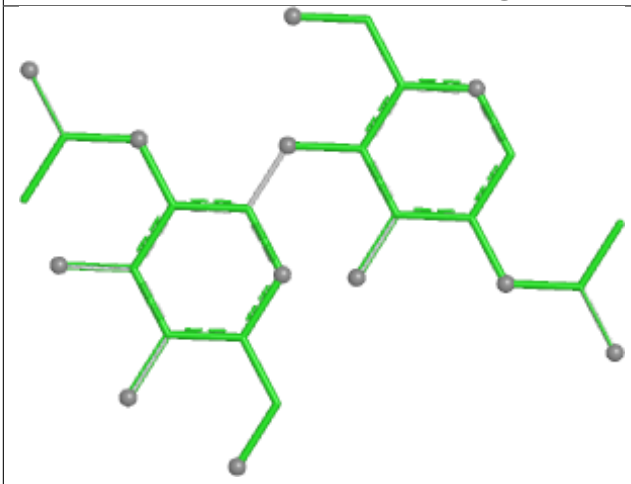


Torsions

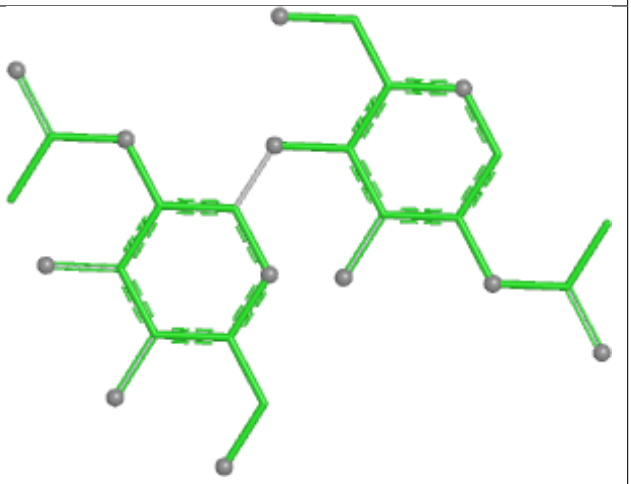


Rings

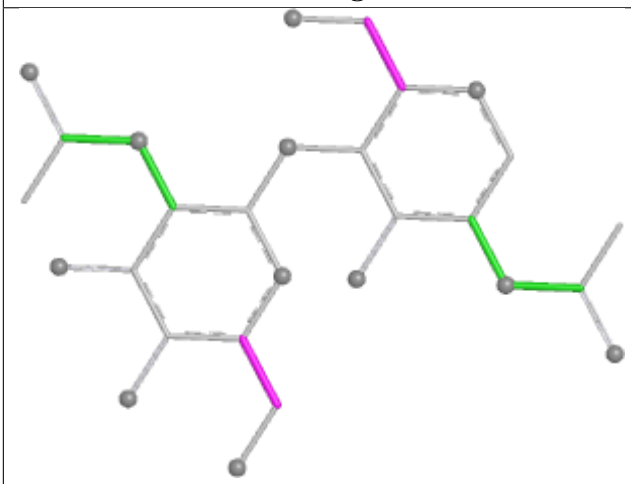
Oligosaccharide Chain P



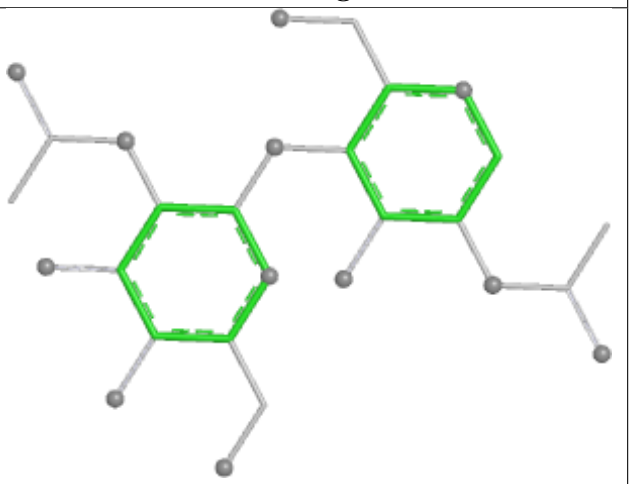
Bond lengths



Bond angles

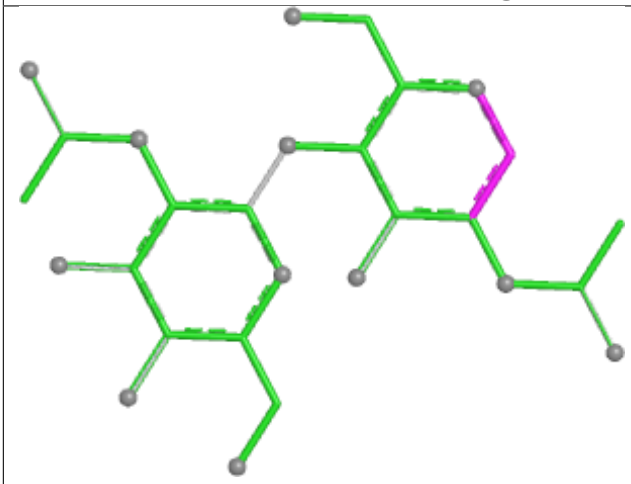


Torsions

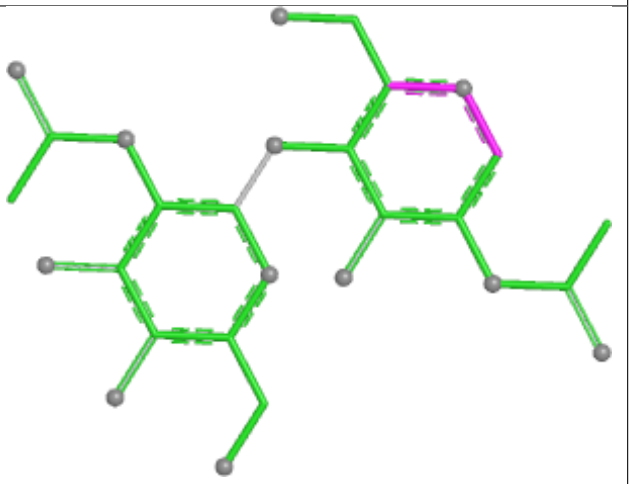


Rings

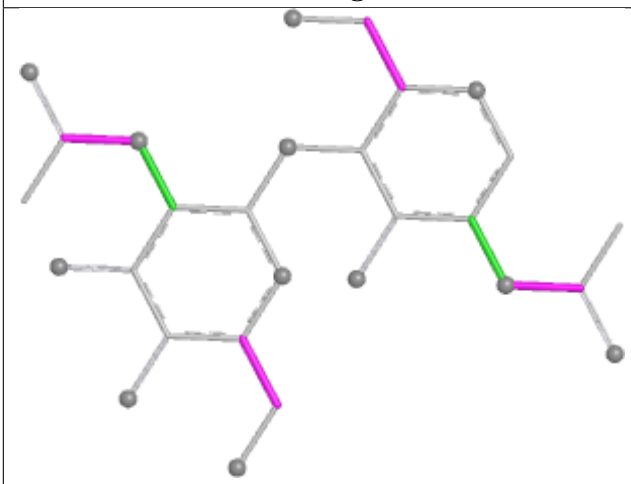
Oligosaccharide Chain S



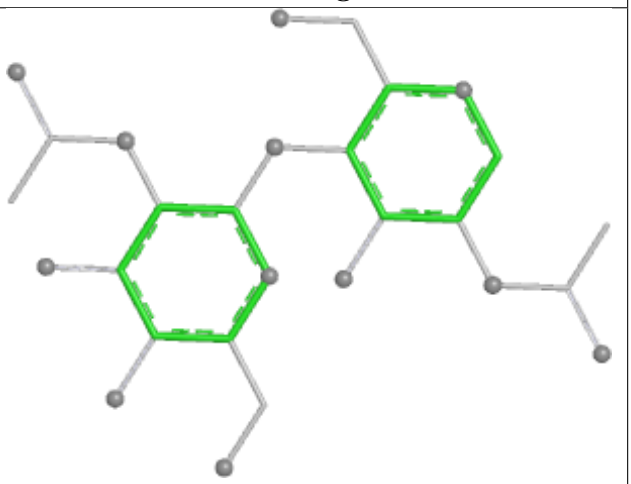
Bond lengths



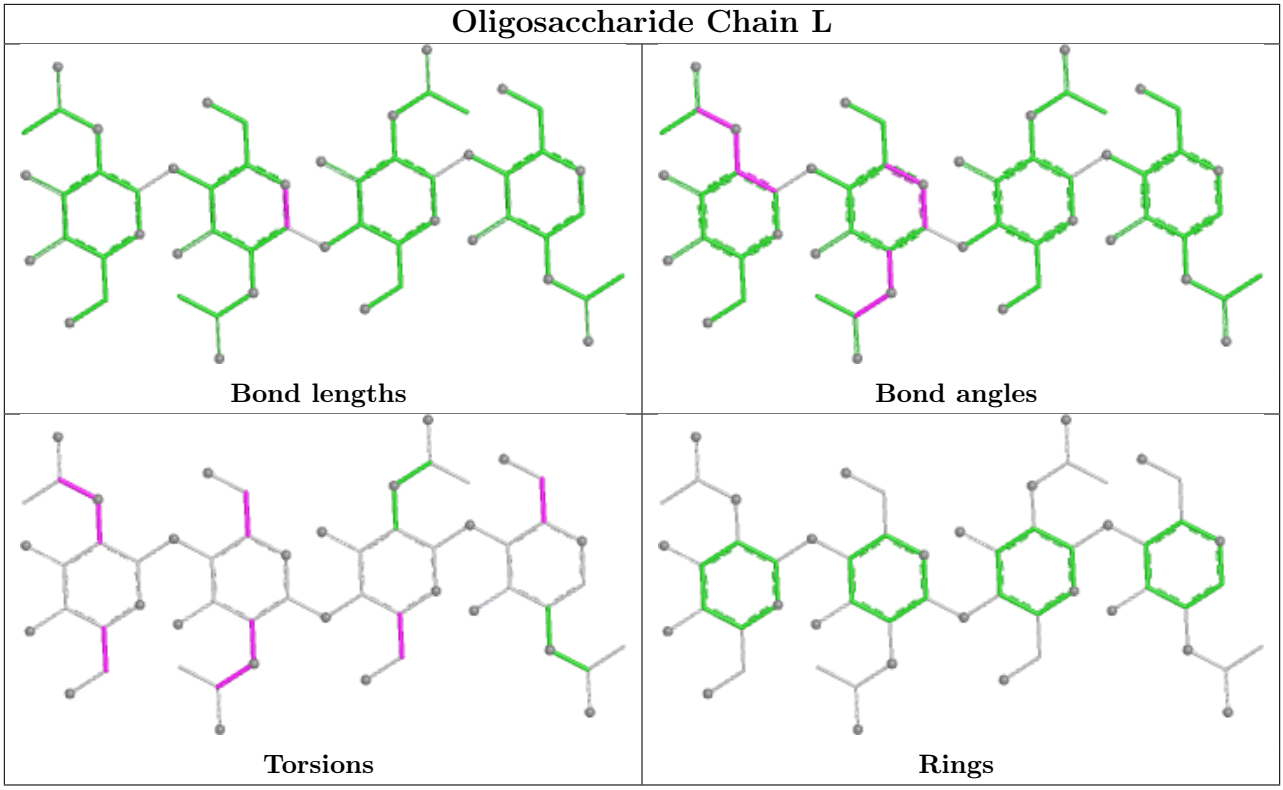
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	NAG	D	1201	3	14,14,15	0.39	0	17,19,21	0.49	0
11	CLR	A	2405	-	31,31,31	1.07	3 (9%)	48,48,48	1.41	11 (22%)
10	Y01	A	2403	-	38,38,38	2.53	12 (31%)	57,57,57	4.51	34 (59%)
11	CLR	A	2404	-	31,31,31	1.11	2 (6%)	48,48,48	1.34	8 (16%)
12	3PE	A	2411	-	50,50,50	0.51	0	53,55,55	0.55	1 (1%)
8	NAG	A	2401	1	14,14,15	0.35	0	17,19,21	0.49	0
8	NAG	D	1202	3	14,14,15	0.87	1 (7%)	17,19,21	0.89	1 (5%)
11	CLR	A	2408	-	31,31,31	1.07	3 (9%)	48,48,48	1.39	9 (18%)
11	CLR	A	2407	-	31,31,31	1.09	2 (6%)	48,48,48	1.36	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	Y01	A	2406	-	38,38,38	2.83	13 (34%)	57,57,57	4.57	33 (57%)
12	3PE	A	2410	-	39,39,50	0.58	0	42,44,55	0.57	1 (2%)
11	CLR	A	2409	-	31,31,31	1.10	2 (6%)	48,48,48	1.31	7 (14%)
13	PT5	A	2412	-	64,64,69	0.85	2 (3%)	79,82,87	1.03	3 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	1201	3	-	2/6/23/26	0/1/1/1
11	CLR	A	2405	-	-	2/10/68/68	0/4/4/4
10	Y01	A	2403	-	-	8/19/77/77	0/4/4/4
11	CLR	A	2404	-	-	7/10/68/68	0/4/4/4
12	3PE	A	2411	-	-	25/54/54/54	-
8	NAG	A	2401	1	-	2/6/23/26	0/1/1/1
8	NAG	D	1202	3	-	2/6/23/26	0/1/1/1
11	CLR	A	2408	-	-	6/10/68/68	0/4/4/4
11	CLR	A	2407	-	-	7/10/68/68	0/4/4/4
10	Y01	A	2406	-	-	13/19/77/77	0/4/4/4
12	3PE	A	2410	-	-	8/43/43/54	-
11	CLR	A	2409	-	-	8/10/68/68	0/4/4/4
13	PT5	A	2412	-	-	25/61/85/90	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2406	Y01	CAK-CBD	11.35	1.71	1.53
10	A	2403	Y01	CAK-CBD	8.78	1.67	1.53
10	A	2406	Y01	CBD-CBG	-6.47	1.41	1.53
10	A	2403	Y01	CBD-CBG	-6.19	1.42	1.53
10	A	2403	Y01	CAI-CAZ	4.62	1.42	1.33
10	A	2406	Y01	CAI-CAZ	4.54	1.42	1.33
13	A	2412	PT5	O18-C11	4.15	1.45	1.33
13	A	2412	PT5	O16-C10	3.87	1.45	1.34
10	A	2403	Y01	CAU-CBI	-3.77	1.47	1.54
10	A	2403	Y01	CAK-CAI	-3.61	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2406	Y01	CAU-CBI	-3.59	1.47	1.54
10	A	2406	Y01	CAL-CAX	3.52	1.58	1.50
10	A	2406	Y01	CAK-CAI	-3.48	1.43	1.50
10	A	2403	Y01	CAL-CAX	3.38	1.58	1.50
10	A	2406	Y01	CAV-CBC	3.22	1.59	1.52
10	A	2403	Y01	CAV-CAZ	-3.20	1.45	1.51
10	A	2406	Y01	CAV-CAZ	-2.96	1.45	1.51
10	A	2403	Y01	CBB-CBE	-2.67	1.49	1.54
10	A	2406	Y01	CBB-CBE	-2.66	1.49	1.54
8	D	1202	NAG	O5-C1	2.53	1.47	1.43
10	A	2403	Y01	CAE-CBI	2.49	1.58	1.54
10	A	2403	Y01	CAV-CBC	2.42	1.57	1.52
10	A	2406	Y01	CBH-CBF	-2.39	1.52	1.56
11	A	2404	CLR	C18-C13	-2.36	1.50	1.54
11	A	2407	CLR	C18-C13	-2.35	1.50	1.54
10	A	2403	Y01	CBH-CBF	-2.30	1.52	1.56
11	A	2409	CLR	C18-C13	-2.28	1.50	1.54
11	A	2408	CLR	C18-C13	-2.27	1.50	1.54
11	A	2405	CLR	C18-C13	-2.26	1.50	1.54
11	A	2404	CLR	C7-C6	2.16	1.54	1.50
11	A	2405	CLR	C8-C14	-2.14	1.49	1.53
10	A	2403	Y01	CBH-CAZ	-2.08	1.48	1.52
10	A	2406	Y01	CAE-CBI	2.08	1.57	1.54
11	A	2408	CLR	C8-C14	-2.07	1.49	1.53
10	A	2406	Y01	OAW-CAY	2.06	1.40	1.34
11	A	2407	CLR	C7-C6	2.06	1.54	1.50
11	A	2409	CLR	C7-C6	2.05	1.54	1.50
10	A	2406	Y01	CBH-CAZ	-2.05	1.49	1.52
11	A	2405	CLR	C16-C17	2.03	1.58	1.54
11	A	2408	CLR	C16-C17	2.03	1.58	1.54

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2406	Y01	CAD-CBH-CAT	12.11	127.85	109.43
10	A	2403	Y01	CAD-CBH-CAT	11.72	127.26	109.43
10	A	2403	Y01	CAD-CBH-CAZ	-10.07	92.99	108.38
10	A	2403	Y01	CAK-CBD-CBG	-9.83	97.02	110.93
10	A	2406	Y01	CAD-CBH-CAZ	-9.60	93.72	108.38
10	A	2406	Y01	CBI-CBE-CBB	-8.77	105.95	119.50
10	A	2403	Y01	CAQ-CBG-CBD	-8.51	105.52	119.10
10	A	2403	Y01	CBI-CBE-CBB	-8.39	106.55	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	2403	Y01	CAV-CAZ-CBH	-8.35	105.73	116.42
10	A	2403	Y01	CBH-CBF-CBD	-8.33	100.54	112.71
10	A	2406	Y01	CBI-CBG-CBD	-8.19	102.78	114.41
10	A	2406	Y01	CAV-CAZ-CAI	8.06	131.50	120.57
10	A	2406	Y01	CAQ-CBG-CBD	-7.84	106.60	119.10
10	A	2403	Y01	CAV-CAZ-CAI	7.74	131.05	120.57
10	A	2406	Y01	CAT-CBH-CBF	-7.72	98.52	108.74
10	A	2406	Y01	CBH-CBF-CBD	-7.20	102.19	112.71
10	A	2403	Y01	CAT-CBH-CBF	-7.11	99.33	108.74
10	A	2406	Y01	CAK-CBD-CBF	6.97	117.78	109.72
10	A	2403	Y01	CBG-CBI-CBE	-6.90	92.18	100.10
10	A	2406	Y01	CAV-CAZ-CBH	-6.33	108.32	116.42
10	A	2406	Y01	CAP-CAQ-CBG	-6.25	92.91	105.14
10	A	2406	Y01	CAK-CBD-CBG	-6.23	102.12	110.93
10	A	2403	Y01	CBI-CBG-CBD	-6.12	105.72	114.41
10	A	2406	Y01	CBG-CBI-CBE	-5.84	93.40	100.10
10	A	2406	Y01	CAE-CBI-CAU	-5.70	102.20	110.61
10	A	2403	Y01	CBD-CAK-CAI	-5.51	105.13	112.76
10	A	2403	Y01	CAE-CBI-CBE	5.36	121.40	111.68
10	A	2403	Y01	CAP-CAQ-CBG	-5.29	94.80	105.14
10	A	2406	Y01	OAW-CAY-CAM	5.25	122.83	111.48
10	A	2406	Y01	CBF-CBD-CBG	-5.22	102.26	109.09
10	A	2403	Y01	CAE-CBI-CAU	-5.20	102.94	110.61
10	A	2403	Y01	OAW-CAY-CAM	5.07	122.45	111.48
10	A	2406	Y01	CBD-CAK-CAI	-5.02	105.80	112.76
10	A	2406	Y01	CBF-CBH-CAZ	-5.00	102.34	109.65
10	A	2406	Y01	CAD-CBH-CBF	4.99	117.26	111.66
10	A	2403	Y01	CAC-CBB-CAO	4.92	117.95	110.34
10	A	2406	Y01	CAE-CBI-CBE	4.82	120.42	111.68
10	A	2406	Y01	CAC-CBB-CAO	4.68	117.59	110.34
10	A	2403	Y01	CAK-CBD-CBF	4.56	114.99	109.72
10	A	2403	Y01	OAW-CBC-CAV	4.36	117.01	108.04
10	A	2406	Y01	CAU-CAS-CBF	-4.28	105.85	113.14
10	A	2403	Y01	CAS-CAU-CBI	-4.25	105.56	112.74
13	A	2412	PT5	O16-C10-C12	4.18	120.52	111.48
10	A	2406	Y01	CAS-CAU-CBI	-4.11	105.81	112.74
10	A	2406	Y01	OAW-CBC-CAV	4.06	116.40	108.04
10	A	2406	Y01	CAT-CBH-CAZ	3.80	115.30	108.74
10	A	2406	Y01	OAW-CAY-OAG	-3.72	115.01	123.70
10	A	2403	Y01	CAS-CBF-CBD	3.70	116.94	111.78
10	A	2403	Y01	OAW-CAY-OAG	-3.65	115.17	123.70
8	D	1202	NAG	C1-O5-C5	3.40	116.74	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2405	CLR	C22-C20-C17	-3.36	103.36	110.33
10	A	2406	Y01	CAO-CBB-CBE	-3.33	103.44	110.33
10	A	2406	Y01	CAR-CAT-CBH	-3.26	105.84	112.78
10	A	2406	Y01	CAS-CBF-CBH	3.19	117.02	113.08
11	A	2408	CLR	C22-C20-C17	-3.19	103.72	110.33
10	A	2403	Y01	CAU-CAS-CBF	-3.16	107.77	113.14
10	A	2403	Y01	CAO-CBB-CBE	-3.16	103.79	110.33
10	A	2406	Y01	CAQ-CBG-CBI	3.13	107.52	103.84
10	A	2403	Y01	CBF-CBD-CBG	-3.13	105.00	109.09
10	A	2403	Y01	CAT-CBH-CAZ	3.02	113.95	108.74
13	A	2412	PT5	C8-O16-C10	-2.90	110.86	117.80
10	A	2403	Y01	CAQ-CBG-CBI	2.89	107.23	103.84
11	A	2407	CLR	C22-C20-C17	-2.83	104.45	110.33
11	A	2404	CLR	C16-C17-C13	-2.82	100.53	103.84
13	A	2412	PT5	O18-C11-C31	2.82	120.42	111.83
10	A	2403	Y01	CAU-CBI-CBG	2.74	111.34	107.25
11	A	2404	CLR	C13-C17-C20	-2.73	115.28	119.50
10	A	2403	Y01	CAC-CBB-CBE	-2.72	108.80	112.88
10	A	2403	Y01	CAD-CBH-CBF	2.65	114.64	111.66
11	A	2409	CLR	C13-C17-C20	-2.62	115.44	119.50
11	A	2404	CLR	C18-C13-C12	2.59	114.43	110.61
10	A	2406	Y01	CAC-CBB-CBE	-2.57	109.02	112.88
11	A	2405	CLR	C16-C17-C20	-2.50	108.40	112.18
12	A	2410	3PE	O12-P-O14	2.49	124.00	112.44
11	A	2408	CLR	C13-C17-C20	-2.48	115.66	119.50
11	A	2407	CLR	C18-C13-C12	2.48	114.26	110.61
12	A	2411	3PE	O12-P-O14	2.44	123.81	112.44
11	A	2409	CLR	C22-C20-C17	-2.44	105.28	110.33
11	A	2408	CLR	C18-C13-C12	2.43	114.18	110.61
11	A	2404	CLR	C7-C8-C14	-2.38	107.56	110.93
11	A	2405	CLR	C12-C13-C14	-2.37	103.70	107.25
11	A	2409	CLR	C18-C13-C12	2.36	114.08	110.61
10	A	2406	Y01	CAU-CBI-CBG	2.35	110.76	107.25
11	A	2407	CLR	C13-C17-C20	-2.32	115.91	119.50
11	A	2405	CLR	C18-C13-C12	2.29	113.98	110.61
11	A	2408	CLR	C12-C13-C14	-2.29	103.82	107.25
11	A	2408	CLR	C21-C20-C22	-2.28	106.82	110.34
11	A	2404	CLR	C11-C12-C13	-2.27	108.91	112.74
11	A	2409	CLR	C7-C8-C14	-2.27	107.72	110.93
11	A	2408	CLR	C24-C23-C22	-2.26	103.15	113.28
11	A	2407	CLR	C19-C10-C9	-2.25	109.14	111.66
10	A	2403	Y01	CAP-CBE-CBI	2.25	106.48	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2405	CLR	C21-C20-C22	-2.24	106.87	110.34
11	A	2408	CLR	C10-C5-C6	2.23	126.19	122.93
11	A	2405	CLR	C10-C5-C6	2.23	126.18	122.93
11	A	2409	CLR	C11-C12-C13	-2.21	109.00	112.74
10	A	2403	Y01	CAR-CBC-CAV	-2.19	107.93	110.97
11	A	2407	CLR	C21-C20-C22	-2.16	107.00	110.34
11	A	2405	CLR	C13-C17-C20	-2.15	116.18	119.50
11	A	2409	CLR	C16-C17-C13	-2.14	101.32	103.84
10	A	2403	Y01	CAR-CAT-CBH	-2.14	108.23	112.78
11	A	2405	CLR	C24-C23-C22	-2.12	103.76	113.28
11	A	2407	CLR	C11-C12-C13	-2.10	109.19	112.74
11	A	2405	CLR	C19-C10-C9	-2.10	109.30	111.66
11	A	2407	CLR	C24-C23-C22	-2.10	103.87	113.28
11	A	2409	CLR	C24-C23-C22	-2.10	103.89	113.28
11	A	2404	CLR	C19-C10-C9	-2.09	109.31	111.66
11	A	2404	CLR	C17-C13-C14	-2.09	97.70	100.10
10	A	2406	Y01	CAP-CBE-CBI	2.07	106.28	103.84
11	A	2408	CLR	C19-C10-C9	-2.06	109.35	111.66
11	A	2405	CLR	C7-C8-C14	-2.06	108.02	110.93
11	A	2404	CLR	C24-C23-C22	-2.03	104.16	113.28
11	A	2408	CLR	C7-C8-C14	-2.03	108.06	110.93
11	A	2407	CLR	C12-C13-C14	-2.02	104.22	107.25
11	A	2407	CLR	C7-C8-C14	-2.02	108.08	110.93
11	A	2405	CLR	C1-C2-C3	2.01	113.14	110.48
10	A	2403	Y01	CAP-CBE-CBB	2.00	115.21	112.18

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	2403	Y01	OAG-CAY-OAW-CBC
10	A	2403	Y01	CAX-CAL-CAM-CAY
10	A	2406	Y01	OAG-CAY-OAW-CBC
10	A	2406	Y01	CAM-CAY-OAW-CBC
12	A	2410	3PE	C1-O11-P-O12
12	A	2410	3PE	C1-O11-P-O13
12	A	2410	3PE	O21-C2-C3-O31
12	A	2411	3PE	C1-O11-P-O13
12	A	2411	3PE	C1-O11-P-O14
12	A	2411	3PE	C11-O13-P-O12
12	A	2411	3PE	O13-C11-C12-N
12	A	2411	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
13	A	2412	PT5	C7-O13-P1-O11
13	A	2412	PT5	C7-O13-P1-O1
13	A	2412	PT5	C1-O1-P1-O13
13	A	2412	PT5	O19-C11-O18-C9
12	A	2411	3PE	O32-C31-O31-C3
11	A	2404	CLR	C13-C17-C20-C21
11	A	2404	CLR	C13-C17-C20-C22
12	A	2411	3PE	C32-C31-O31-C3
13	A	2412	PT5	C31-C11-O18-C9
8	A	2401	NAG	O5-C5-C6-O6
10	A	2403	Y01	CAM-CAY-OAW-CBC
12	A	2411	3PE	C22-C21-O21-C2
11	A	2404	CLR	C16-C17-C20-C21
11	A	2409	CLR	C13-C17-C20-C21
10	A	2406	Y01	CAX-CAL-CAM-CAY
8	D	1202	NAG	O5-C5-C6-O6
13	A	2412	PT5	C12-C10-O16-C8
13	A	2412	PT5	O17-C10-O16-C8
11	A	2404	CLR	C21-C20-C22-C23
11	A	2409	CLR	C21-C20-C22-C23
11	A	2404	CLR	C17-C20-C22-C23
11	A	2408	CLR	C17-C20-C22-C23
11	A	2409	CLR	C17-C20-C22-C23
8	A	2401	NAG	C4-C5-C6-O6
8	D	1202	NAG	C4-C5-C6-O6
11	A	2408	CLR	C21-C20-C22-C23
11	A	2409	CLR	C13-C17-C20-C22
11	A	2407	CLR	C21-C20-C22-C23
11	A	2407	CLR	C17-C20-C22-C23
13	A	2412	PT5	C10-C12-C13-C14
10	A	2403	Y01	CAN-CAJ-CAO-CBB
11	A	2404	CLR	C20-C22-C23-C24
10	A	2406	Y01	CAN-CAJ-CAO-CBB
11	A	2407	CLR	C20-C22-C23-C24
12	A	2411	3PE	C25-C26-C27-C28
10	A	2403	Y01	CAJ-CAN-CBA-CAB
10	A	2406	Y01	CAO-CBB-CBE-CBI
10	A	2403	Y01	CAJ-CAN-CBA-CAA
10	A	2406	Y01	CAJ-CAN-CBA-CAA
11	A	2405	CLR	C20-C22-C23-C24
12	A	2411	3PE	C2B-C2C-C2D-C2E
10	A	2406	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
11	A	2409	CLR	C16-C17-C20-C21
11	A	2408	CLR	C22-C23-C24-C25
13	A	2412	PT5	C31-C32-C33-C34
12	A	2411	3PE	C2A-C2B-C2C-C2D
10	A	2406	Y01	CAJ-CAO-CBB-CAC
11	A	2407	CLR	C13-C17-C20-C21
11	A	2404	CLR	C16-C17-C20-C22
10	A	2406	Y01	CAC-CBB-CBE-CBI
13	A	2412	PT5	C32-C33-C34-C35
13	A	2412	PT5	C12-C13-C14-C15
13	A	2412	PT5	C25-C26-C27-C28
11	A	2409	CLR	C22-C23-C24-C25
12	A	2411	3PE	C27-C28-C29-C2A
13	A	2412	PT5	C27-C28-C29-C30
12	A	2410	3PE	C1-C2-C3-O31
12	A	2411	3PE	O11-C1-C2-O21
13	A	2412	PT5	C15-C16-C17-C18
13	A	2412	PT5	C16-C17-C18-C19
13	A	2412	PT5	C21-C22-C23-C24
12	A	2411	3PE	C24-C25-C26-C27
12	A	2410	3PE	C37-C38-C39-C3A
12	A	2411	3PE	O11-C1-C2-C3
13	A	2412	PT5	C9-C8-O16-C10
10	A	2406	Y01	CAO-CBB-CBE-CAP
11	A	2409	CLR	C16-C17-C20-C22
12	A	2411	3PE	C32-C33-C34-C35
12	A	2411	3PE	C12-C11-O13-P
13	A	2412	PT5	C1-O1-P1-O11
12	A	2411	3PE	C3B-C3C-C3D-C3E
13	A	2412	PT5	C39-C40-C41-C42
11	A	2409	CLR	C23-C24-C25-C27
12	A	2411	3PE	O21-C2-C3-O31
11	A	2407	CLR	C13-C17-C20-C22
13	A	2412	PT5	C35-C36-C37-C38
11	A	2408	CLR	C13-C17-C20-C21
8	D	1201	NAG	C3-C2-N2-C7
12	A	2410	3PE	C1-O11-P-O14
12	A	2411	3PE	C1-O11-P-O12
12	A	2411	3PE	C11-O13-P-O11
10	A	2406	Y01	CAC-CBB-CBE-CAP
12	A	2410	3PE	C38-C39-C3A-C3B
12	A	2411	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
11	A	2407	CLR	C16-C17-C20-C21
11	A	2407	CLR	C23-C24-C25-C26
13	A	2412	PT5	C24-C25-C26-C27
12	A	2411	3PE	C2F-C2G-C2H-C2I
11	A	2408	CLR	C20-C22-C23-C24
13	A	2412	PT5	C8-C7-O13-P1
8	D	1201	NAG	C1-C2-N2-C7
11	A	2408	CLR	C23-C24-C25-C27
10	A	2403	Y01	CAM-CAL-CAX-OAH
12	A	2411	3PE	C3D-C3E-C3F-C3G
10	A	2403	Y01	CAM-CAL-CAX-OAF
12	A	2411	3PE	C1-C2-C3-O31
12	A	2410	3PE	C22-C23-C24-C25
13	A	2412	PT5	C1-O1-P1-O12
10	A	2406	Y01	CAL-CAM-CAY-OAW
13	A	2412	PT5	C4-O4-P4-O41
11	A	2405	CLR	C13-C17-C20-C21
10	A	2406	Y01	CAL-CAM-CAY-OAG
13	A	2412	PT5	C6-C1-O1-P1

There are no ring outliers.

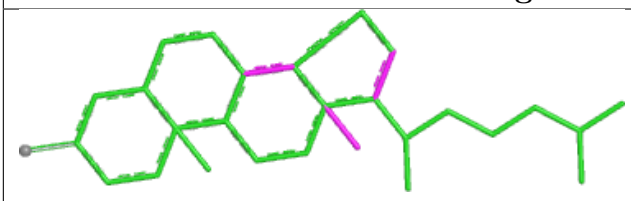
10 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2405	CLR	2	0
10	A	2403	Y01	11	0
11	A	2404	CLR	3	0
12	A	2411	3PE	4	0
8	D	1202	NAG	1	0
11	A	2408	CLR	4	0
10	A	2406	Y01	5	0
12	A	2410	3PE	1	0
11	A	2409	CLR	2	0
13	A	2412	PT5	12	0

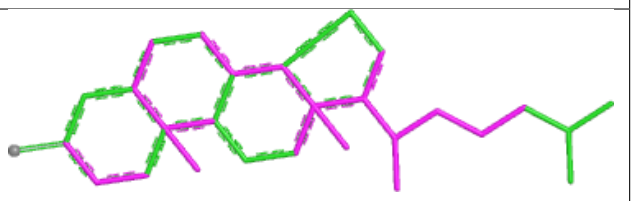
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

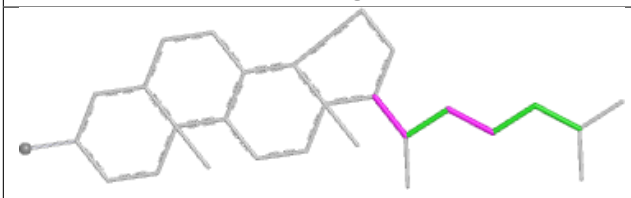
Ligand CLR A 2405



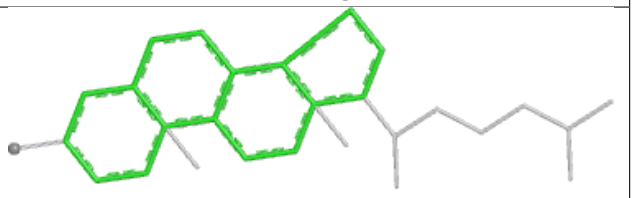
Bond lengths



Bond angles

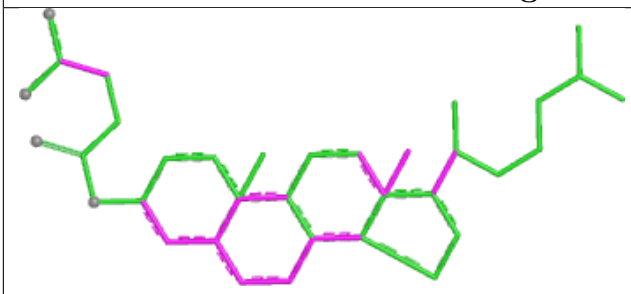


Torsions

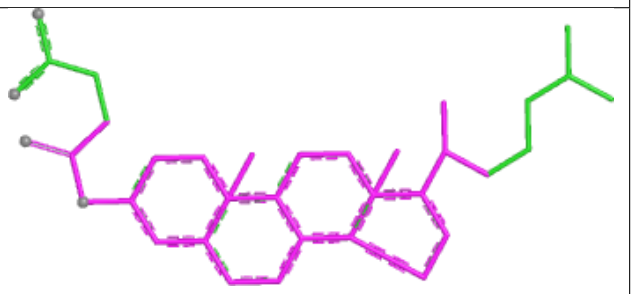


Rings

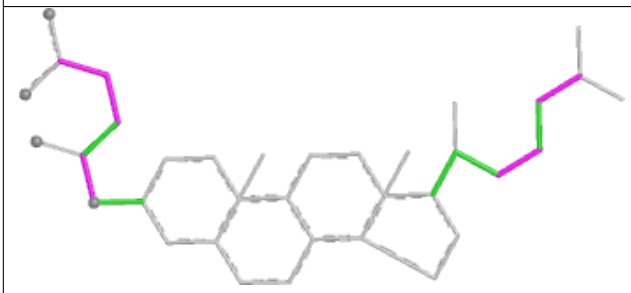
Ligand Y01 A 2403



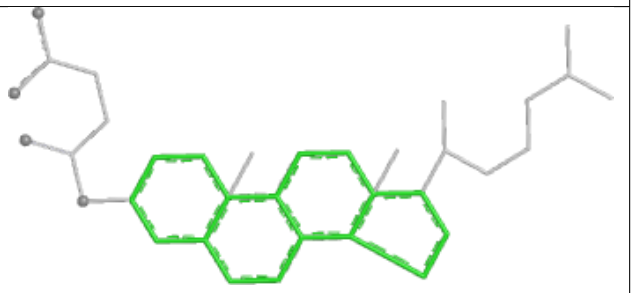
Bond lengths



Bond angles

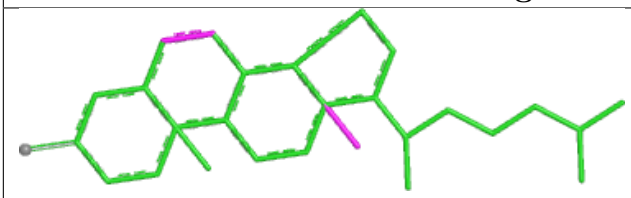


Torsions

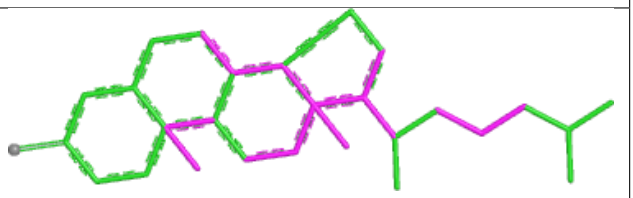


Rings

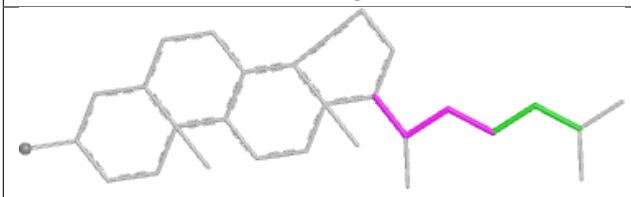
Ligand CLR A 2404



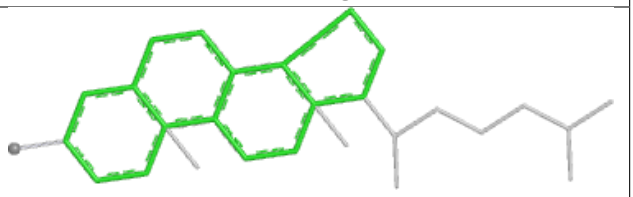
Bond lengths



Bond angles

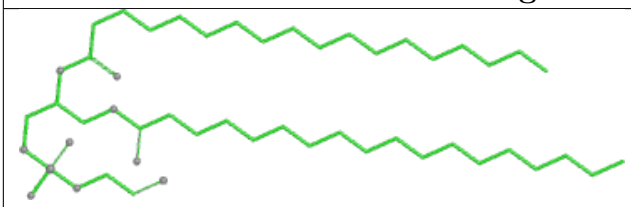


Torsions

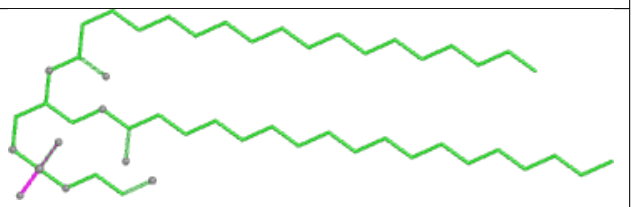


Rings

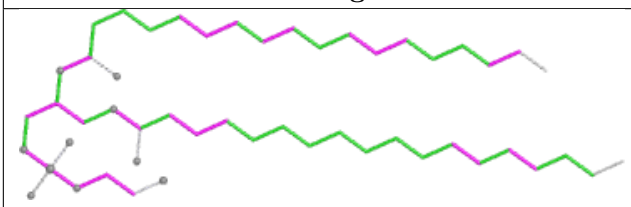
Ligand 3PE A 2411



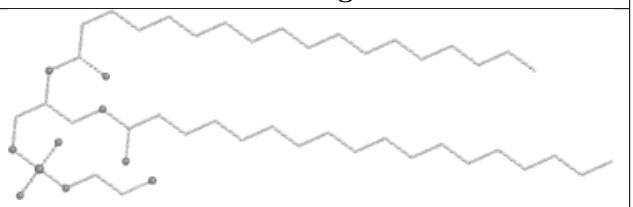
Bond lengths



Bond angles

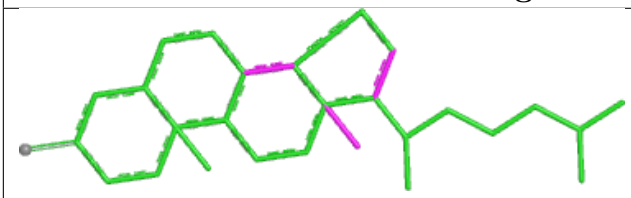


Torsions

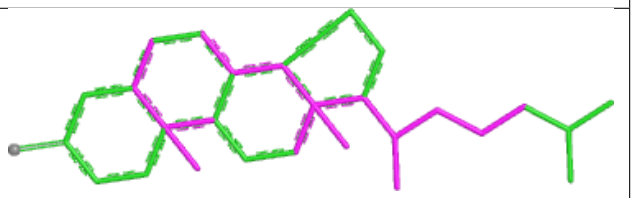


Rings

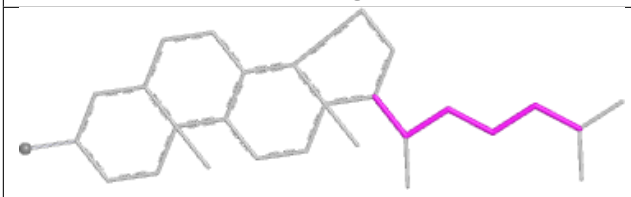
Ligand CLR A 2408



Bond lengths



Bond angles



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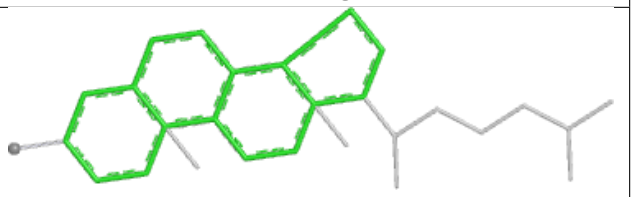
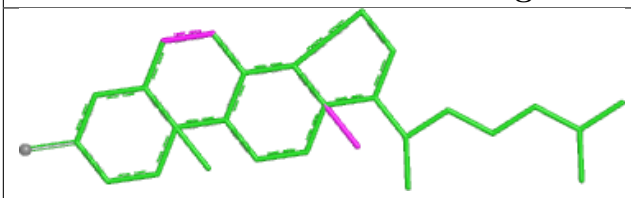
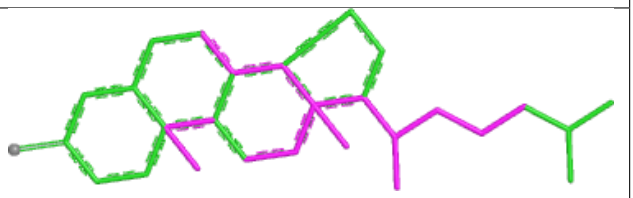


Rings

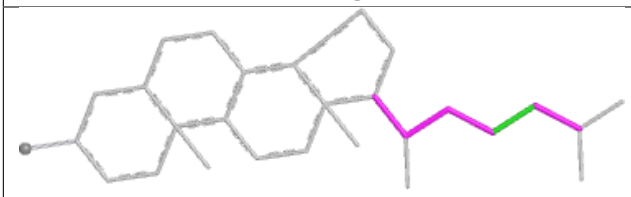
Ligand CLR A 2407



Bond lengths



Bond angles



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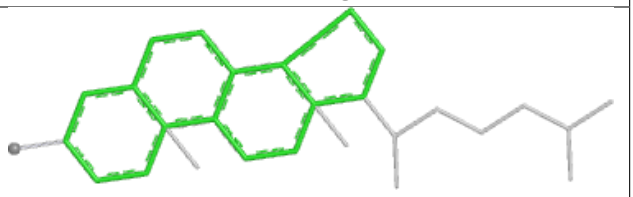
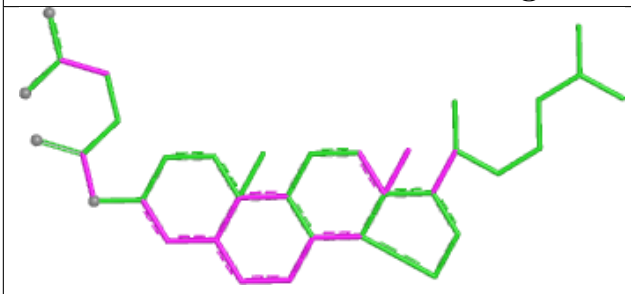
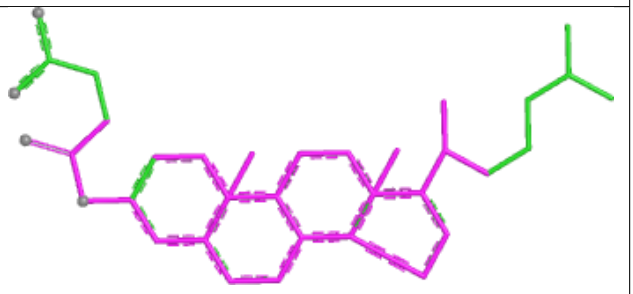


Rings

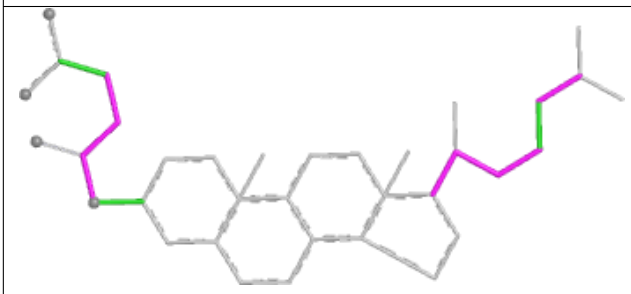
Ligand Y01 A 2406



Bond lengths



Bond angles



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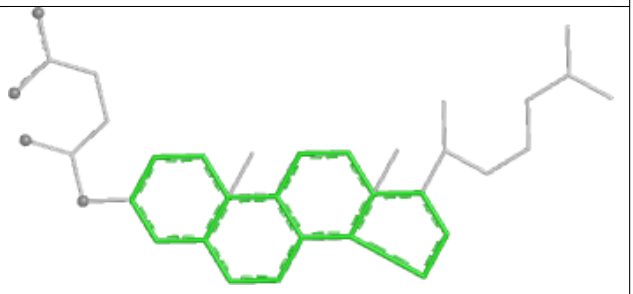
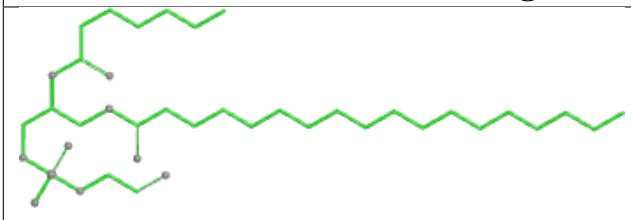


Rings

Ligand 3PE A 2410



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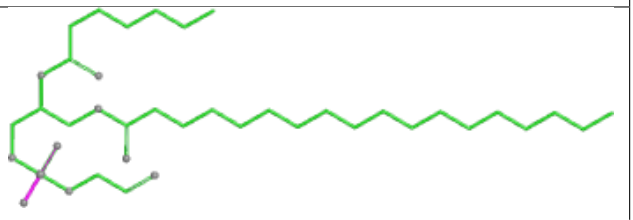
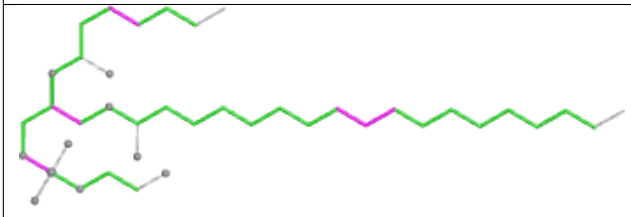
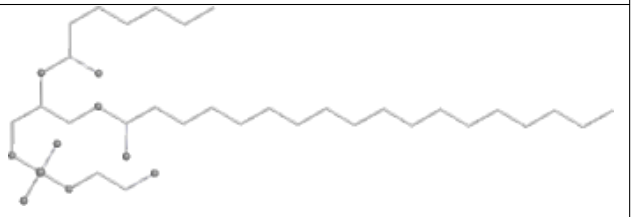


Bond angles

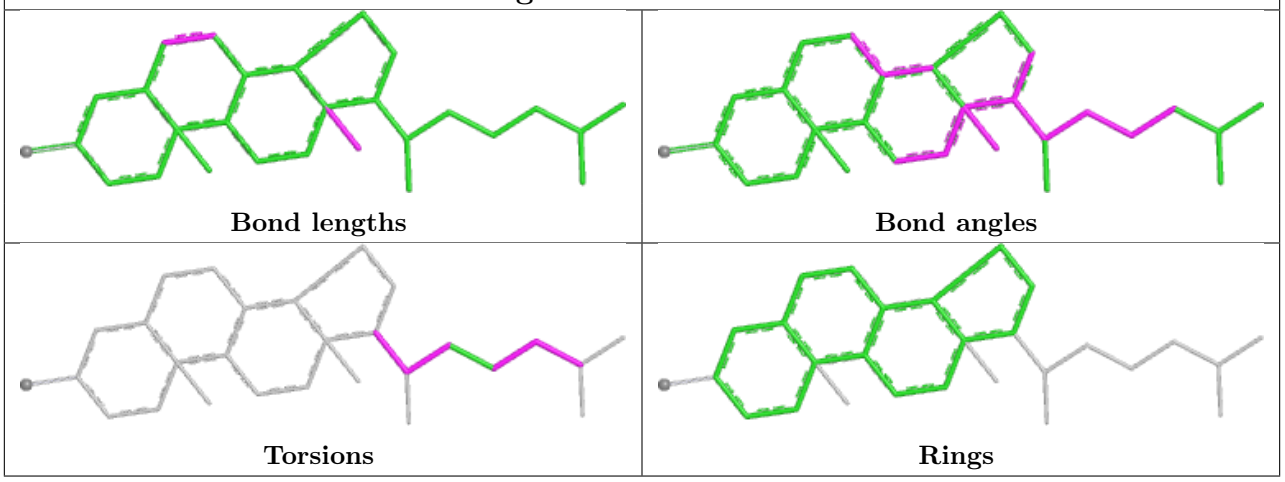


Torsions

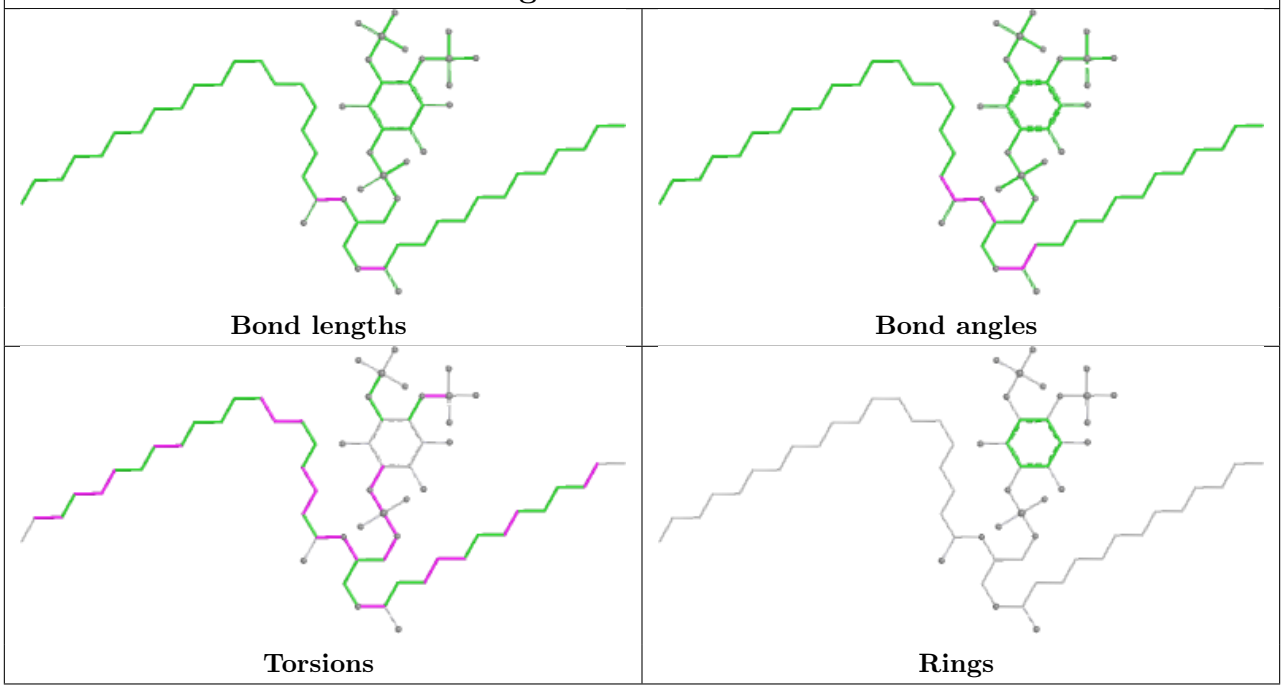


Rings

Ligand CLR A 2409



Ligand PT5 A 2412



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.

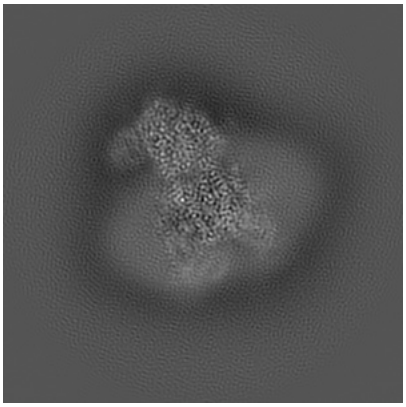
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23867. These allow visual inspection of the internal detail of the map and identification of artifacts.

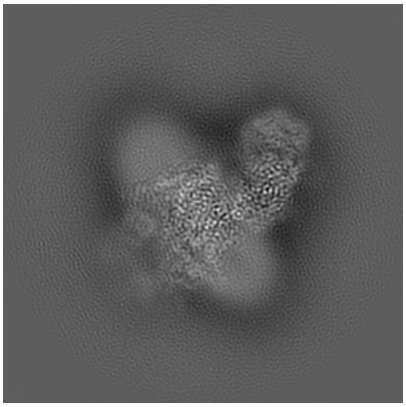
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

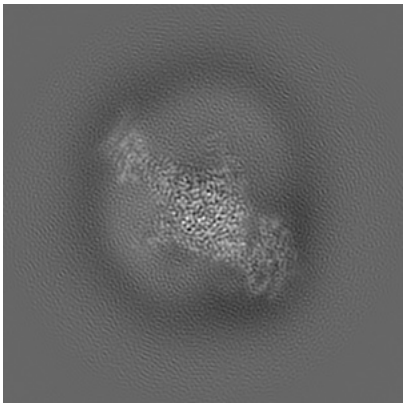
6.1.1 Primary map



X



Y

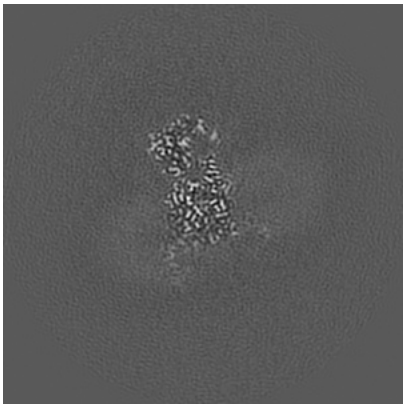


Z

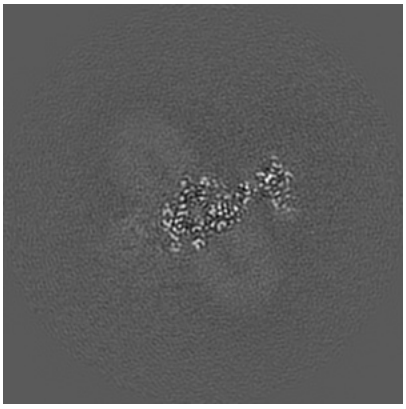
The images above show the map projected in three orthogonal directions.

6.2 Central slices

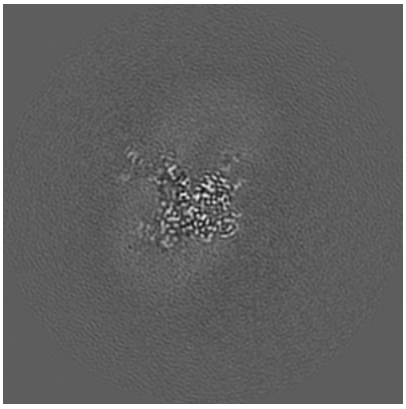
6.2.1 Primary map



X Index: 140



Y Index: 140

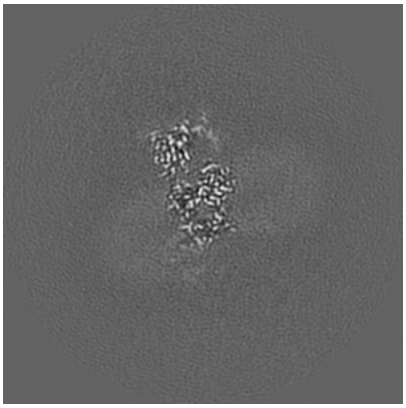


Z Index: 140

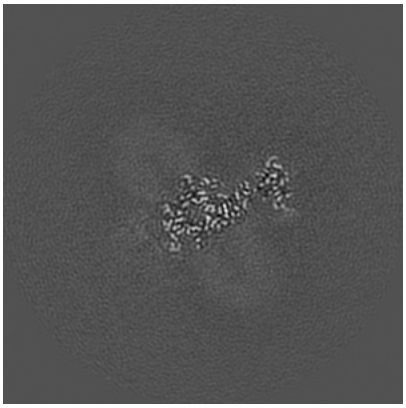
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

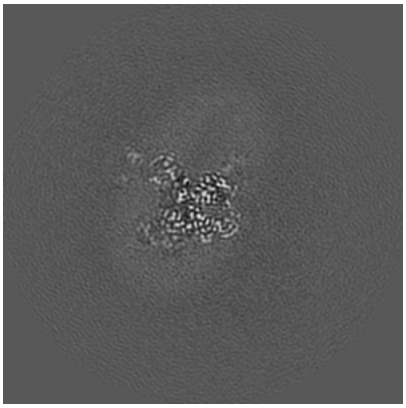
6.3.1 Primary map



X Index: 136



Y Index: 141

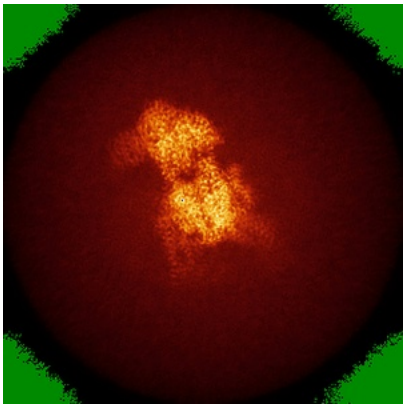


Z Index: 141

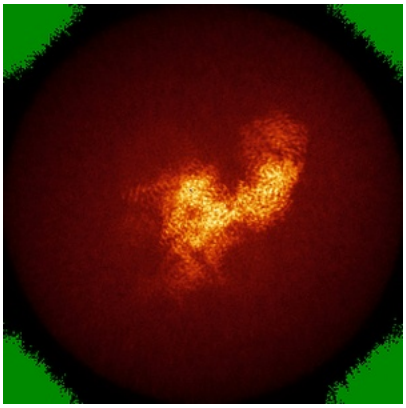
The images above show the largest variance slices of the map in three orthogonal directions.

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

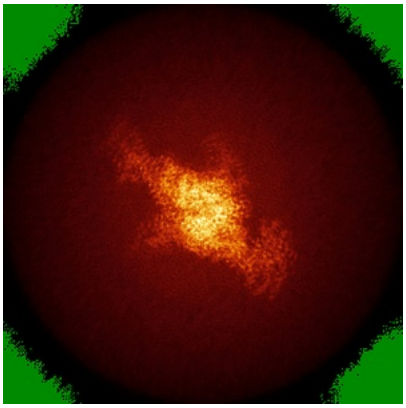
6.4.1 Primary map



X



Y



Z

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

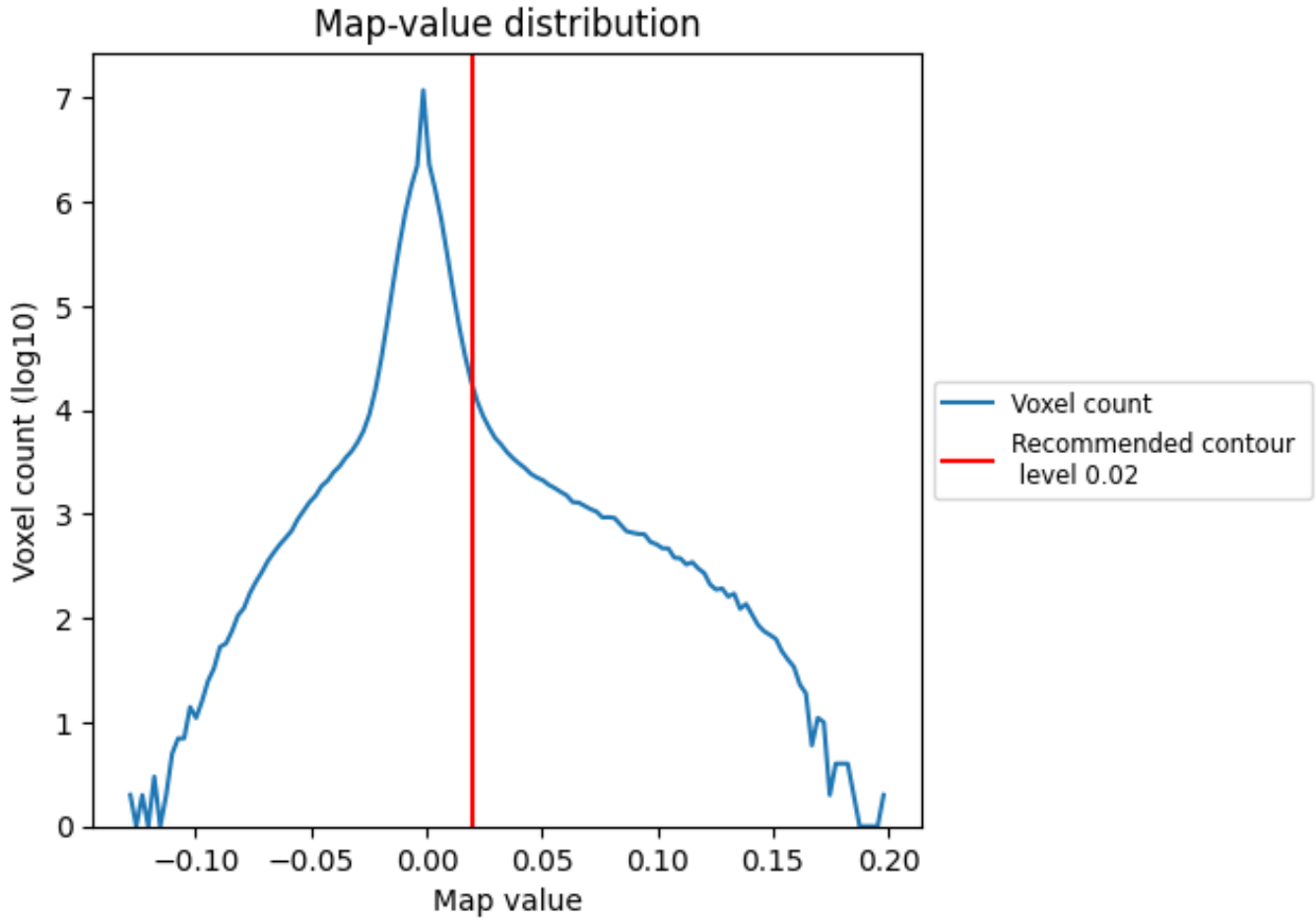
6.6 Mask visualisation (i)

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

7 Map analysis

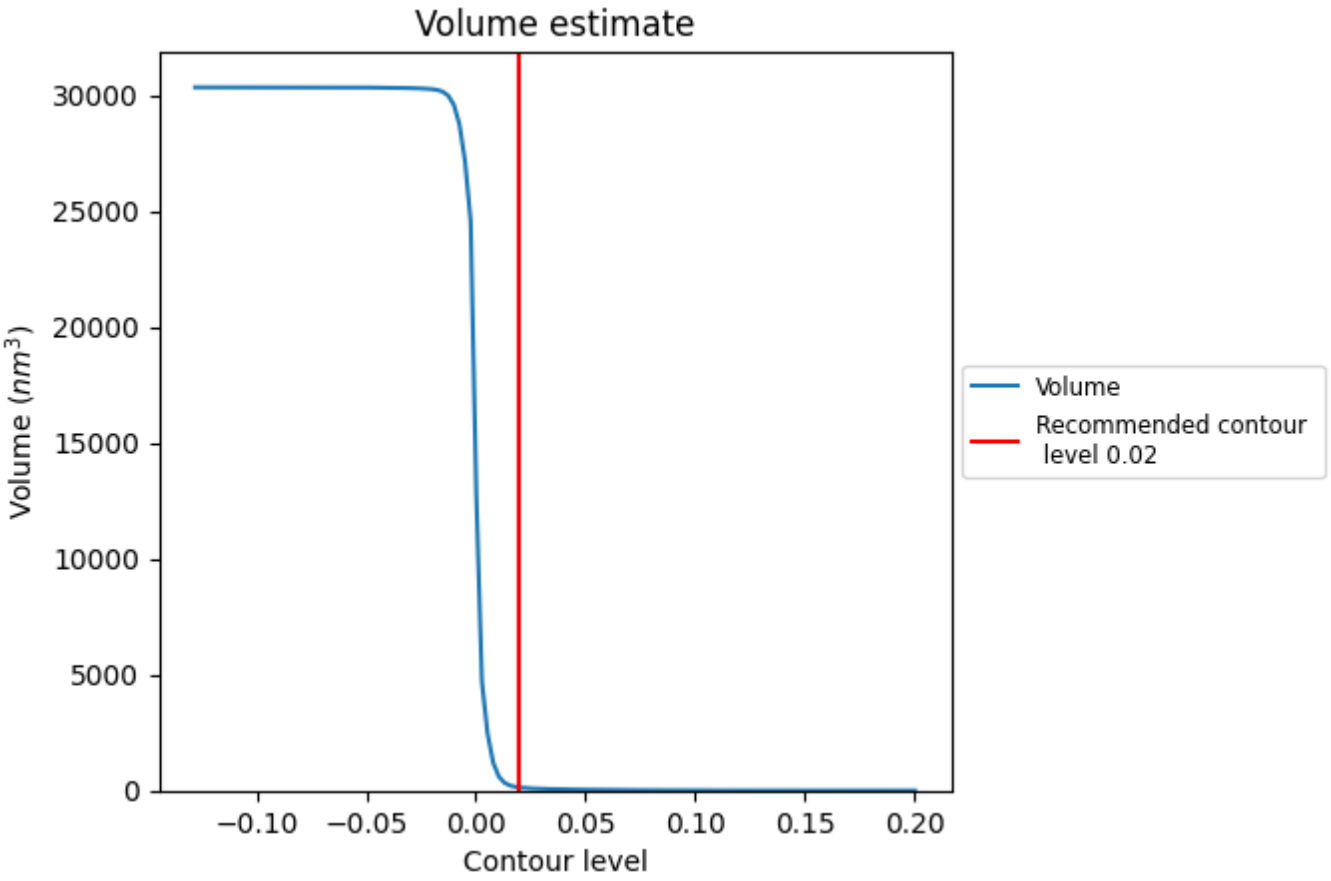
This section contains the results of statistical analysis of the map.

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.

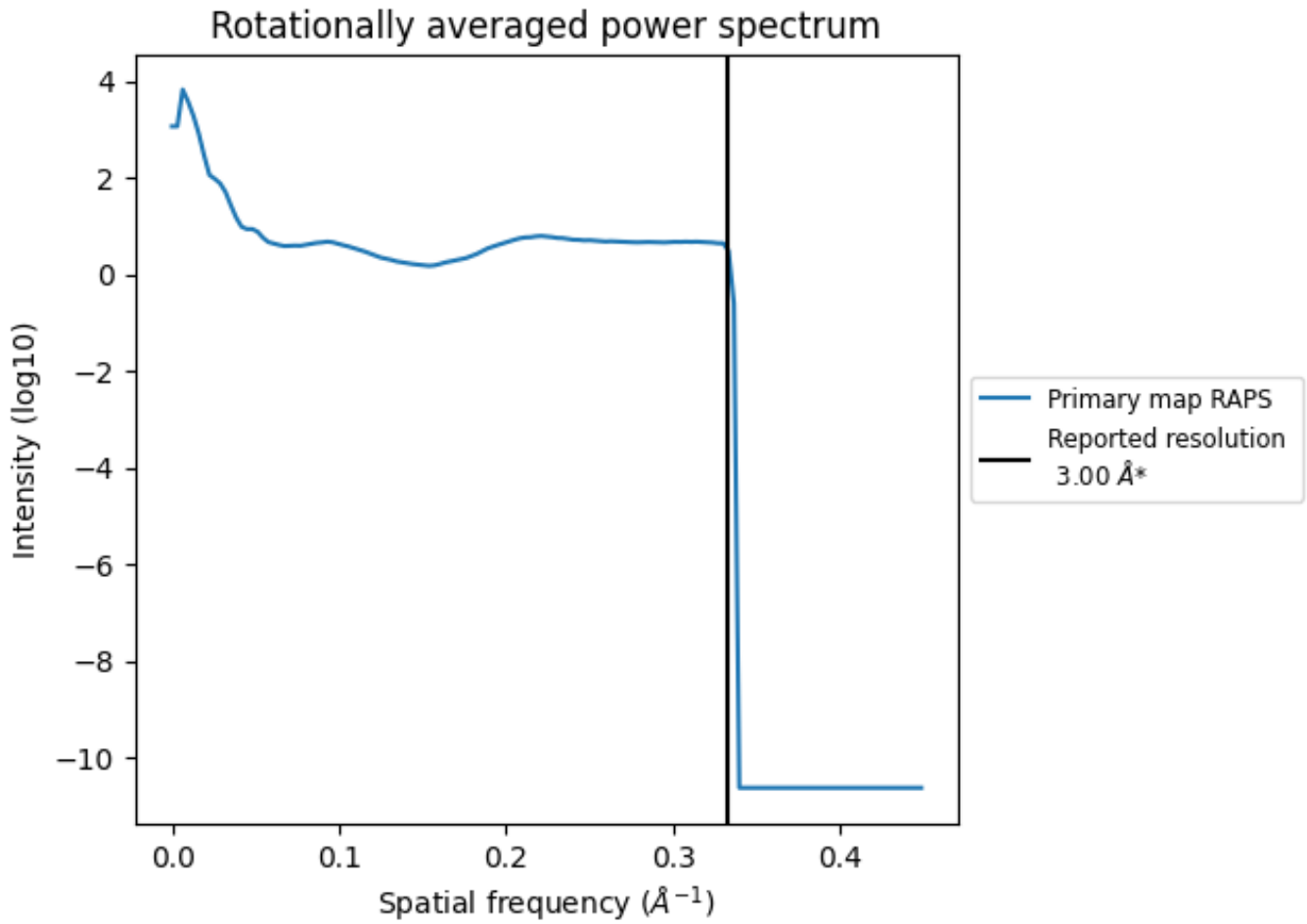
7.2 Volume estimate



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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}

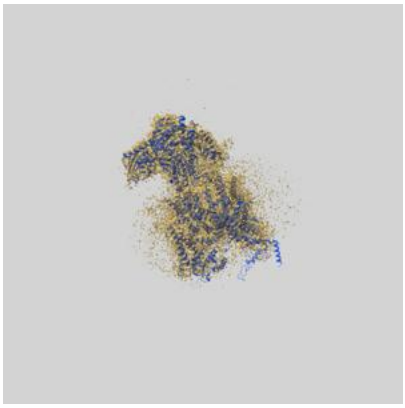
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

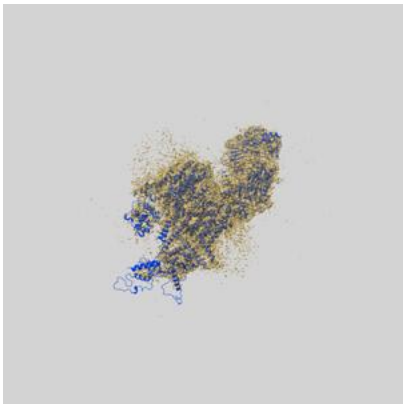
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23867 and PDB model 7MIX. Per-residue inclusion information can be found in section 3 on page 10.

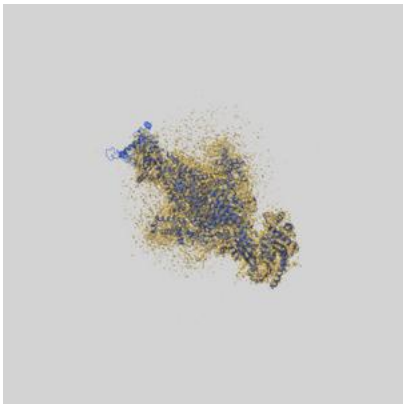
9.1 Map-model overlay



X



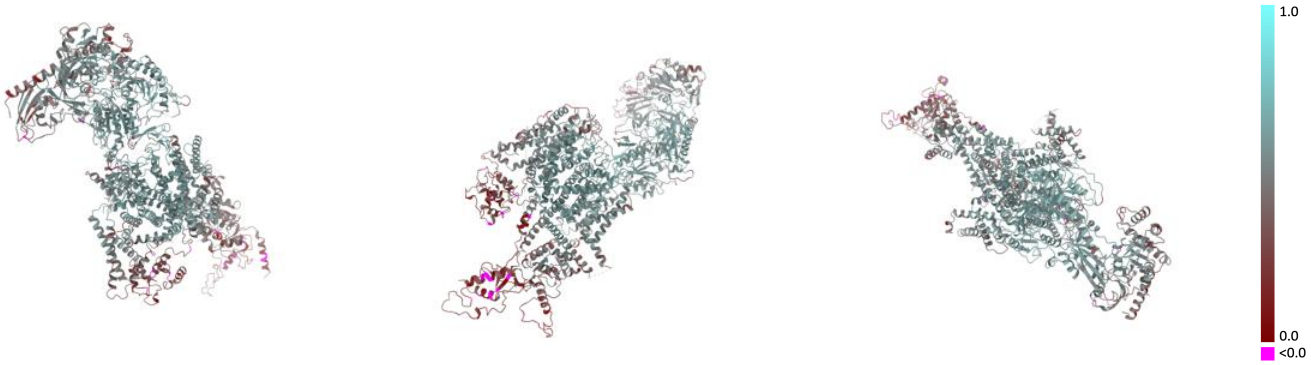
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

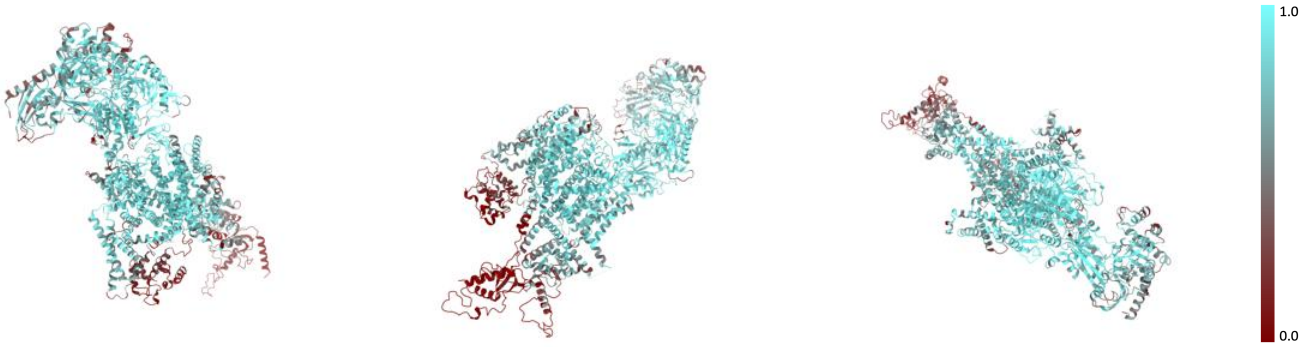
9.2 Q-score mapped to coordinate model (i)



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.

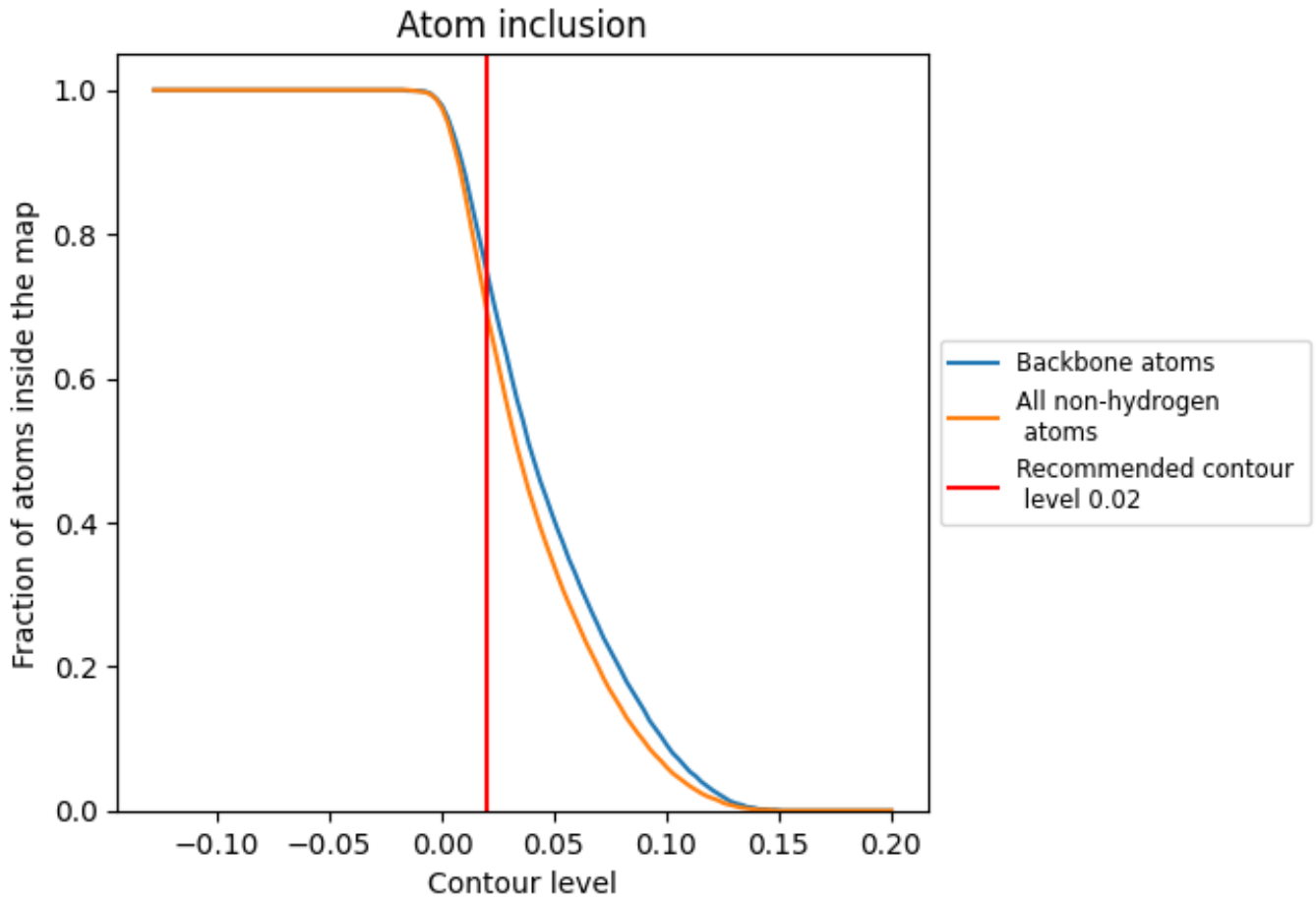
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.4960
A	0.7230	0.5090
B	0.9180	0.6050
C	0.2910	0.3270
D	0.7880	0.5320
G	0.5000	0.3530
J	0.2860	0.3440
L	0.7140	0.4910
P	0.4290	0.3640
S	0.4640	0.3820