



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 06:08 AM JST

PDB ID : 7VFU
EMDB ID : EMD-31959
Title : Human N-type voltage gated calcium channel CaV2.2-alpha2/delta1-beta1 complex, bound to ziconotide
Authors : Dong, Y.; Gao, Y.; Wang, Y.; Zhao, Y.
Deposited on : 2021-09-13
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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

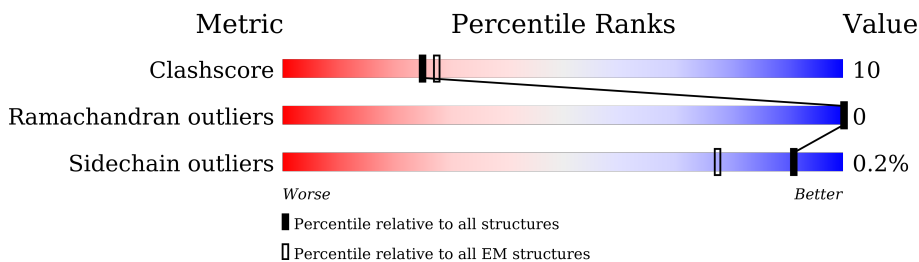
1 Overall quality at a glance

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 $\leq 5\%$. 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	
2	E	25	
3	D	598	
4	B	1103	
5	C	3	
5	F	3	
6	G	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 19946 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
1	A	1266	Total	C	N	O	S	0	0
			10202	6715	1651	1771	65		

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

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

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	163	Total	C	N	O	S	0	0
			1266	802	218	240	6		

- Molecule 4 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

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



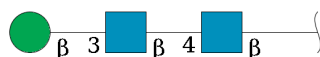
Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	3	Total	C	N	O	0	0
			39	22	2	15		

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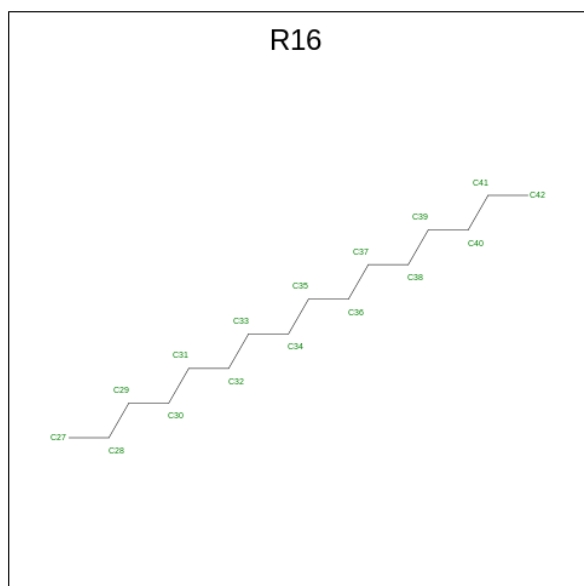
Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 7 is HEXADECANE (three-letter code: R16) (formula: C₁₆H₃₄).



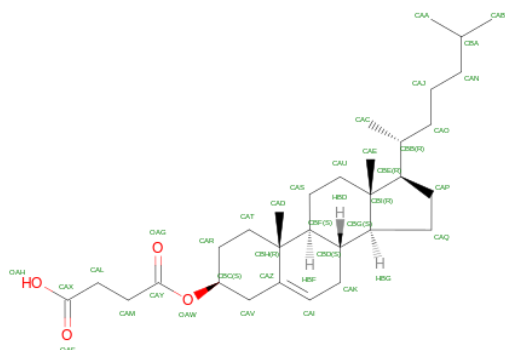
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			16	16	
7	A	1	Total	C	0
			16	16	

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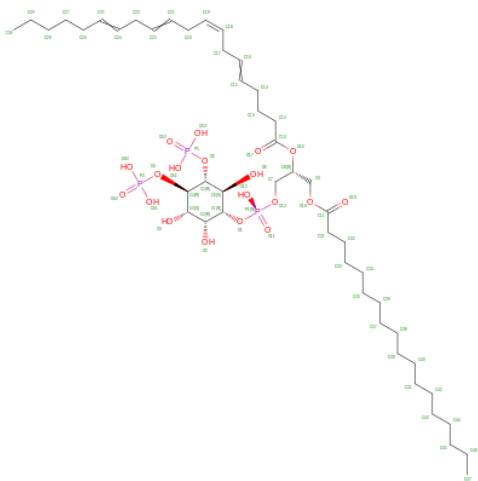
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0
7	A	1	Total C 11 11	0
7	A	1	Total C 13 13	0
7	A	1	Total C 15 15	0
7	A	1	Total C 13 13	0
7	A	1	Total C 12 12	0
7	A	1	Total C 15 15	0
7	A	1	Total C 13 13	0
7	A	1	Total C 16 16	0
7	A	1	Total C 16 16	0

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



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

- Molecule 9 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).

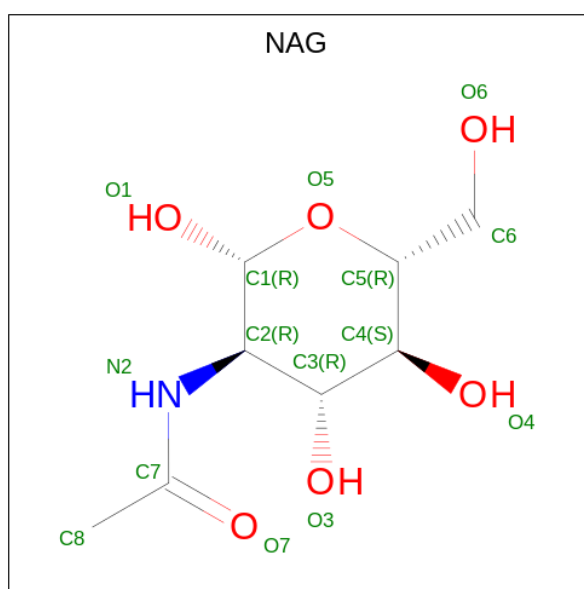


Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	O	P	0
			61	39	19	3	

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Ca	0
			2	2	

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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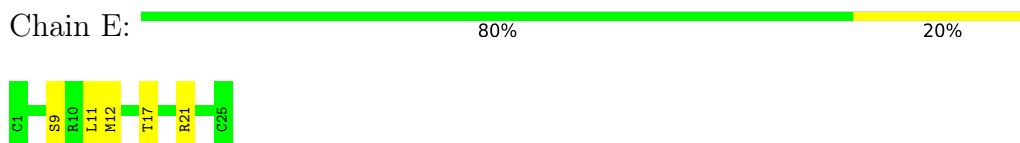
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	14	8	1	5	0



[illegible]

- Molecule 2: Omega-conotoxin MVIIA



- Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1

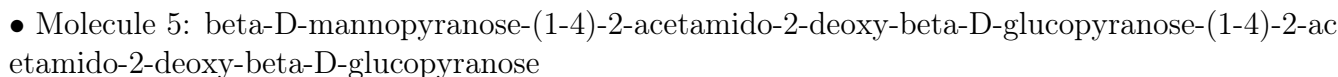
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VAL	GLN	GLY	VAL	ALA	ILE	THR	PHE	GLU	PRO	LYS	ASP	PHE	LEU	HIS	LYS	ILE	GLU	LYS	TYR	ASN	ASN	ASP	TRP	TRP	ILE	GLY	ARG	LEU	VAL	LYS	GLU	GLY	CYS	CYS	GLU	VAL	GLY	PHE	ILE	ILE	PRO	PRO	SER	SER	ASP	LEU	ARG	LEU	LEU	GLN	GLN	GLN	GLN	ASN	ARG
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[illegible][illegible]

ARG ASN LYS ALA ARG TYR CYS ALA GLU GLY GLY GLY PRO VAL LEU LEU GLY ARG ASN LYS ASN GLU LEU GLU GLY TRP GLY ARG GLY VAL TYR ILE ARG

Chain B:



Chain C:





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

Chain F:
67% 33%



- Molecule 6: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:
67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9.6	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	5.227	Depositor
Minimum map value	-3.187	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, Y01, PT5, R16, BMA

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	0.28	0/10448	0.43	0/14152
2	E	0.31	0/176	0.52	0/228
3	D	0.31	0/1287	0.48	1/1741 (0.1%)
4	B	0.31	0/7799	0.48	0/10578
All	All	0.30	0/19710	0.45	1/26699 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	261	ASP	CB-CG-OD2	5.24	123.01	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10202	0	10179	210	0
2	E	176	0	176	6	0
3	D	1266	0	1259	46	0
4	B	7637	0	7426	159	0
5	C	39	0	34	0	0
5	F	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	39	0	34	0	0
7	A	268	0	542	9	0
8	A	105	0	147	11	0
9	A	61	0	61	4	0
10	A	2	0	0	0	0
11	B	112	0	104	3	0
All	All	19946	0	19996	413	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 10.

All (413) 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:D:235:VAL:CG1	3:D:377:LEU:CD2	2.39	1.01
3:D:235:VAL:HG12	3:D:377:LEU:CD2	1.92	0.99
3:D:235:VAL:HG12	3:D:377:LEU:HD23	1.41	0.98
3:D:235:VAL:CG1	3:D:377:LEU:HD21	1.96	0.94
1:A:473:PHE:HB3	1:A:477:ARG:HH22	1.39	0.87
3:D:235:VAL:CG1	3:D:377:LEU:HD23	2.05	0.83
1:A:323:THR:O	1:A:332:ASN:ND2	2.13	0.81
4:B:149:PHE:HB3	4:B:158:GLN:HB3	1.65	0.78
4:B:85:ASP:HB3	4:B:500:LEU:HD22	1.65	0.78
4:B:994:LEU:HB3	4:B:1001:ARG:HB2	1.66	0.78
1:A:1334:VAL:HG23	4:B:233:ILE:HG21	1.65	0.78
1:A:1350:ASN:HD21	8:A:2404:Y01:HAD1	1.52	0.75
4:B:104:ALA:HB2	4:B:189:LEU:HD21	1.71	0.72
1:A:119:PRO:HD2	4:B:263:SER:HA	1.71	0.71
1:A:122:ASP:HB2	4:B:262:GLY:HA3	1.72	0.71
1:A:108:ASN:HD21	1:A:198:ARG:HH11	1.35	0.71
4:B:508:PRO:HG2	4:B:764:TYR:HE2	1.56	0.71
1:A:363:ARG:NH1	1:A:714:ASN:OD1	2.25	0.70
1:A:473:PHE:HB3	1:A:477:ARG:NH2	2.05	0.70
1:A:122:ASP:HB2	4:B:262:GLY:CA	2.23	0.69
1:A:1650:ARG:NH1	1:A:1655:GLU:O	2.25	0.69
1:A:639:ASP:O	4:B:267:LEU:HB2	1.92	0.68
1:A:1262:ILE:HG13	1:A:1268:LEU:HG	1.77	0.67
4:B:508:PRO:HG2	4:B:764:TYR:CE2	2.29	0.67
1:A:307:VAL:O	1:A:311:ILE:HG12	1.96	0.66
4:B:644:TYR:O	4:B:647:THR:OG1	2.13	0.66
1:A:1628:ASP:O	2:E:21:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:751:ASN:O	4:B:753:GLN:NE2	2.30	0.65
3:D:272:ASP:OD1	3:D:274:SER:OG	2.14	0.65
1:A:1174:ARG:NH1	1:A:1177:SER:OG	2.30	0.65
1:A:1173:VAL:HG13	1:A:1174:ARG:HG3	1.79	0.65
3:D:381:PRO:HG2	3:D:384:MET:HG2	1.78	0.65
1:A:395:ALA:HB2	3:D:251:ALA:HB2	1.80	0.64
4:B:90:LEU:HD12	4:B:615:THR:HG21	1.80	0.64
4:B:57:LEU:HD23	4:B:798:VAL:HG11	1.78	0.64
1:A:673:ILE:HD11	1:A:686:SER:HB3	1.81	0.63
4:B:224:VAL:HG23	4:B:225:ASP:H	1.63	0.63
4:B:646:GLU:HA	4:B:649:LYS:NZ	2.13	0.63
4:B:204:LEU:HD13	4:B:456:LEU:HD13	1.81	0.63
1:A:230:LEU:HD11	1:A:311:ILE:HG21	1.81	0.62
1:A:1403:PHE:HB2	1:A:1404:PRO:HD3	1.81	0.62
4:B:368:ARG:HG2	4:B:398:PRO:HB3	1.80	0.62
4:B:423:THR:HG23	4:B:426:TYR:HE2	1.63	0.62
1:A:1163:SER:HB2	1:A:1257:ARG:HH11	1.65	0.62
1:A:1334:VAL:CG2	4:B:233:ILE:HG21	2.29	0.61
4:B:105:GLU:OE2	4:B:442:LYS:NZ	2.33	0.61
4:B:237:ASP:OD2	4:B:424:GLN:NE2	2.32	0.61
4:B:721:SER:O	4:B:724:LYS:HE3	2.01	0.60
1:A:1233:ALA:HB2	1:A:1250:LEU:HB3	1.83	0.60
1:A:1630:THR:O	2:E:21:ARG:NH2	2.35	0.60
1:A:1291:LEU:O	1:A:1295:ILE:HD12	2.02	0.59
4:B:36:TRP:HH2	4:B:829:SER:HA	1.66	0.59
1:A:1323:ARG:O	4:B:173:TYR:HB2	2.03	0.59
4:B:775:PHE:CD1	4:B:794:VAL:HG22	2.37	0.59
1:A:380:GLN:NE2	1:A:725:MET:SD	2.76	0.59
1:A:642:PRO:HB3	2:E:11:LEU:HB3	1.83	0.59
3:D:231:PRO:HD2	3:D:339:PRO:HA	1.84	0.58
3:D:235:VAL:HG11	3:D:377:LEU:CD2	2.32	0.58
1:A:100:MET:O	1:A:104:THR:HG23	2.02	0.58
1:A:229:LEU:HD21	1:A:1585:ILE:HB	1.84	0.58
4:B:885:HIS:O	4:B:889:ILE:HD12	2.03	0.58
4:B:994:LEU:N	4:B:1001:ARG:O	2.30	0.58
1:A:1415:ILE:HG22	1:A:1704:VAL:HG11	1.86	0.57
1:A:374:LYS:O	1:A:378:GLN:HG3	2.03	0.57
1:A:1219:TRP:HE1	1:A:1269:LYS:HE2	1.69	0.57
3:D:232:ILE:HA	3:D:340:ILE:HG22	1.87	0.57
1:A:243:GLU:O	1:A:1568:ARG:NH2	2.38	0.57
3:D:235:VAL:HG13	3:D:377:LEU:HD21	1.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:LYS:NZ	1:A:1273:ASP:OD1	2.37	0.57
3:D:256:LEU:HD21	3:D:401:LEU:HD23	1.86	0.56
4:B:57:LEU:HD13	4:B:715:LEU:HD22	1.87	0.56
4:B:997:GLY:N	4:B:1026:CYS:SG	2.75	0.56
1:A:108:ASN:ND2	1:A:198:ARG:HD3	2.20	0.56
8:A:2412:Y01:HAC1	8:A:2412:Y01:HAU2	1.87	0.56
3:D:265:SER:N	3:D:318:LEU:O	2.35	0.56
1:A:1547:ILE:O	1:A:1551:LEU:HG	2.06	0.56
4:B:226:ASN:HB3	4:B:234:ASP:HB2	1.88	0.56
4:B:646:GLU:HA	4:B:649:LYS:HZ1	1.71	0.56
1:A:1485:THR:HA	1:A:1488:LEU:HD12	1.87	0.56
1:A:1583:TYR:O	1:A:1587:ILE:HD12	2.05	0.56
1:A:1600:PRO:HB2	7:A:2414:R16:H321	1.86	0.55
1:A:1626:LEU:HD13	1:A:1634:ARG:HA	1.88	0.55
1:A:1538:PHE:O	1:A:1542:THR:HG23	2.06	0.55
1:A:104:THR:HG21	1:A:140:ILE:HG21	1.87	0.55
1:A:616:LEU:HD11	1:A:703:VAL:HG21	1.88	0.55
4:B:713:ASN:HA	4:B:716:VAL:HG12	1.87	0.55
1:A:620:ILE:HD12	7:A:2407:R16:H302	1.89	0.55
1:A:1711:PHE:O	1:A:1715:THR:OG1	2.23	0.55
1:A:118:LEU:HD13	4:B:263:SER:HB3	1.88	0.55
4:B:896:LYS:HB3	4:B:977:GLU:OE2	2.06	0.55
1:A:1323:ARG:CZ	4:B:173:TYR:CE2	2.90	0.55
4:B:726:ILE:HB	4:B:729:VAL:HG22	1.87	0.55
1:A:595:LEU:HB3	9:A:2422:PT5:H25	1.87	0.54
3:D:230:ARG:NH2	3:D:386:ASP:OD1	2.37	0.54
4:B:663:PRO:HD3	4:B:756:PRO:HB2	1.89	0.54
4:B:884:ARG:HG3	4:B:1031:LEU:HD11	1.89	0.54
3:D:399:GLU:O	3:D:403:GLU:HG2	2.07	0.54
4:B:772:ASN:HD21	4:B:1011:THR:N	2.05	0.54
1:A:1400:PHE:HA	1:A:1404:PRO:HD2	1.88	0.54
1:A:1690:SER:HA	1:A:1693:PHE:CE1	2.42	0.54
1:A:1728:GLU:O	1:A:1732:VAL:HG23	2.08	0.54
4:B:1042:ASN:ND2	4:B:1045:ASP:OD2	2.39	0.54
1:A:1613:TYR:O	1:A:1687:TYR:OH	2.17	0.54
1:A:317:THR:HG21	1:A:1650:ARG:HG3	1.90	0.53
1:A:1650:ARG:HH11	1:A:1660:ILE:HD11	1.73	0.53
4:B:537:PRO:HB3	4:B:972:GLN:HB2	1.89	0.53
4:B:819:ASN:HA	4:B:822:ILE:HG22	1.89	0.53
1:A:254:PHE:CD2	1:A:284:ARG:HB2	2.43	0.53
3:D:327:ASN:O	3:D:377:LEU:HD11	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:193:PHE:HB3	4:B:218:TYR:HB2	1.91	0.53
1:A:388:TYR:HB3	3:D:355:LEU:HD11	1.90	0.53
4:B:128:LYS:HB3	4:B:227:SER:HA	1.91	0.53
4:B:296:SER:HA	4:B:332:ASP:HB2	1.90	0.53
1:A:712:LEU:HD11	1:A:1410:ILE:HG23	1.89	0.53
1:A:1323:ARG:CZ	4:B:173:TYR:HE2	2.22	0.53
4:B:604:ASN:OD1	11:B:1204:NAG:N2	2.41	0.53
1:A:1214:TYR:CE2	1:A:1220:ASN:HB3	2.43	0.53
4:B:658:TYR:HD2	4:B:749:GLY:HA3	1.73	0.53
1:A:1824:GLU:O	1:A:1828:VAL:HG22	2.08	0.52
1:A:108:ASN:HD21	1:A:198:ARG:NH1	2.05	0.52
1:A:659:ILE:HG23	1:A:665:TRP:HB2	1.91	0.52
4:B:38:ASP:O	4:B:41:GLN:HG3	2.09	0.52
3:D:255:PHE:HD2	3:D:256:LEU:HD22	1.74	0.52
4:B:179:VAL:HG13	4:B:214:LEU:HD21	1.92	0.52
4:B:59:ASP:O	4:B:63:LYS:HB2	2.10	0.52
4:B:285:ASP:O	4:B:309:GLN:NE2	2.37	0.52
7:A:2402:R16:H321	7:A:2403:R16:H302	1.92	0.52
4:B:58:VAL:HG13	4:B:800:ILE:HG22	1.92	0.52
3:D:237:PRO:HG3	3:D:248:MET:HE3	1.92	0.52
4:B:185:TRP:HA	11:B:1208:NAG:H82	1.92	0.52
4:B:494:LEU:HD11	4:B:522:LEU:O	2.10	0.52
4:B:514:ALA:HB3	4:B:522:LEU:HB3	1.92	0.52
1:A:314:GLU:HG3	1:A:665:TRP:CD1	2.45	0.51
1:A:1307:LYS:HB3	1:A:1377:ALA:HB1	1.93	0.51
4:B:363:ASP:OD1	4:B:364:GLY:N	2.41	0.51
1:A:1223:ASP:OD1	1:A:1260:LYS:HE3	2.10	0.51
1:A:1621:PHE:CD1	1:A:1664:CYS:HB3	2.46	0.51
3:D:257:LYS:HB2	3:D:266:ILE:HD12	1.92	0.51
4:B:74:ASN:ND2	4:B:77:GLN:OE1	2.43	0.51
4:B:84:ARG:HG3	11:B:1205:NAG:H81	1.91	0.51
1:A:1688:PHE:O	1:A:1692:ILE:HG12	2.10	0.51
1:A:612:LEU:HD22	1:A:703:VAL:HG13	1.93	0.51
4:B:160:SER:HB3	4:B:220:ALA:HB3	1.91	0.51
4:B:562:LEU:HD12	4:B:1051:ARG:HE	1.76	0.51
1:A:1514:PHE:O	1:A:1517:GLU:HG3	2.11	0.51
4:B:204:LEU:HD11	4:B:493:SER:HB2	1.92	0.51
4:B:667:CYS:HB2	4:B:670:LEU:HD13	1.93	0.51
1:A:1611:PHE:O	1:A:1615:ILE:HG12	2.10	0.51
4:B:481:ASN:OD1	5:F:1:NAG:O6	2.28	0.51
1:A:480:LYS:HE3	1:A:536:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:VAL:HG21	9:A:2422:PT5:H19	1.93	0.51
3:D:260:PHE:HD1	3:D:263:ARG:HH11	1.59	0.51
4:B:103:GLU:HG2	4:B:192:VAL:HG21	1.92	0.51
4:B:407:LYS:HD2	4:B:1068:TYR:CE1	2.46	0.51
1:A:393:PHE:CE1	1:A:476:ARG:HD3	2.46	0.50
1:A:1647:LEU:HD21	1:A:1660:ILE:HG21	1.93	0.50
1:A:320:LEU:HD12	1:A:336:PHE:HB2	1.93	0.50
4:B:63:LYS:HD2	4:B:64:TYR:CZ	2.47	0.50
4:B:647:THR:HG21	4:B:713:ASN:HD22	1.75	0.50
4:B:773:TYR:CE1	4:B:796:LYS:HD2	2.46	0.50
1:A:119:PRO:HA	1:A:633:GLY:O	2.11	0.50
1:A:1318:LEU:HD13	1:A:1320:ARG:HH21	1.77	0.50
1:A:1626:LEU:HD21	1:A:1639:ARG:HD2	1.93	0.50
3:D:305:GLU:OE1	3:D:308:ARG:NH2	2.42	0.50
1:A:1406:PHE:CE2	1:A:1410:ILE:HD11	2.46	0.50
1:A:1526:GLY:H	1:A:1529:ASN:HB2	1.76	0.50
4:B:128:LYS:NZ	4:B:234:ASP:OD2	2.36	0.50
1:A:1840:LEU:O	1:A:1844:HIS:N	2.44	0.50
4:B:100:LEU:HB3	4:B:488:MET:HE2	1.93	0.50
4:B:702:ILE:HA	4:B:705:VAL:HG12	1.92	0.50
1:A:1161:ALA:O	1:A:1165:ILE:HG12	2.11	0.50
4:B:139:GLU:OE2	4:B:173:TYR:OH	2.23	0.50
4:B:167:HIS:CE1	4:B:236:TYR:HD2	2.30	0.50
4:B:511:TYR:OH	4:B:565:GLU:OE2	2.19	0.50
4:B:592:VAL:HG11	4:B:605:ARG:HH21	1.77	0.50
1:A:518:GLU:OE1	1:A:578:ARG:NH2	2.46	0.49
4:B:442:LYS:NZ	4:B:465:PRO:O	2.37	0.49
1:A:275:ARG:HH22	1:A:1634:ARG:HD3	1.78	0.49
4:B:601:ASP:OD1	4:B:602:LYS:N	2.44	0.49
4:B:631:ILE:O	4:B:704:ARG:NH1	2.46	0.49
1:A:90:ARG:HD2	1:A:151:ALA:HB1	1.94	0.49
1:A:1144:HIS:CE1	1:A:1200:ILE:HD13	2.48	0.49
1:A:1490:MET:HB3	1:A:1499:TYR:OH	2.12	0.49
1:A:1549:ASP:HB2	1:A:1567:LEU:HB3	1.95	0.49
4:B:109:ALA:HB2	4:B:469:ILE:HG23	1.95	0.49
1:A:1346:PHE:HB3	1:A:1357:THR:HG23	1.94	0.49
4:B:295:ASN:ND2	4:B:328:LYS:O	2.30	0.49
1:A:1504:LYS:O	1:A:1508:ILE:HG12	2.13	0.48
1:A:319:ILE:O	1:A:323:THR:HG23	2.13	0.48
4:B:37:VAL:HG21	4:B:1006:GLU:HB3	1.94	0.48
4:B:987:SER:HB3	4:B:990:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:147:PRO:HB3	4:B:163:HIS:NE2	2.29	0.48
1:A:301:LEU:HB3	7:A:2410:R16:H322	1.94	0.48
1:A:1521:LYS:HB2	1:A:1530:TYR:HE2	1.78	0.48
7:A:2405:R16:H361	7:A:2405:R16:H423	1.95	0.48
9:A:2422:PT5:H50	9:A:2422:PT5:H42	1.72	0.48
1:A:381:ILE:HD13	3:D:350:LYS:HE3	1.95	0.48
1:A:1721:LEU:HD12	1:A:1802:ALA:HB2	1.95	0.48
4:B:36:TRP:O	4:B:39:LYS:HG2	2.13	0.48
4:B:667:CYS:HA	4:B:697:CYS:CB	2.43	0.48
1:A:715:ALA:O	1:A:719:THR:HG22	2.14	0.48
1:A:1609:LEU:HD22	1:A:1698:LEU:HD22	1.96	0.48
1:A:314:GLU:HG3	1:A:665:TRP:HD1	1.79	0.48
1:A:621:VAL:O	1:A:625:LEU:HG	2.14	0.48
4:B:716:VAL:HG23	4:B:720:TRP:HE3	1.79	0.48
1:A:337:ILE:HD11	1:A:1646:MET:SD	2.54	0.47
1:A:226:ILE:HD12	1:A:350:LEU:HB3	1.97	0.47
1:A:1222:LEU:HD11	1:A:1256:LEU:HD12	1.96	0.47
8:A:2404:Y01:HAP1	8:A:2404:Y01:HAO2	1.63	0.47
1:A:1359:PHE:O	1:A:1363:THR:HG23	2.14	0.47
1:A:1580:ARG:CZ	1:A:1586:ARG:HG2	2.44	0.47
1:A:330:THR:O	1:A:333:TRP:NE1	2.48	0.47
3:D:340:ILE:HD11	3:D:404:TYR:CE2	2.48	0.47
4:B:66:ASP:OD1	4:B:66:ASP:N	2.45	0.47
1:A:1482:ALA:O	1:A:1486:VAL:HG23	2.14	0.47
1:A:1191:THR:O	1:A:1195:THR:HG23	2.15	0.47
3:D:268:ARG:HA	3:D:322:ASP:HB3	1.95	0.47
4:B:261:SER:O	4:B:327:ALA:HB1	2.14	0.47
4:B:709:ALA:O	4:B:742:ARG:NH1	2.45	0.47
1:A:1305:LYS:HE2	1:A:1305:LYS:HB3	1.69	0.47
4:B:710:GLY:O	4:B:714:GLU:HG3	2.15	0.47
1:A:296:ASN:ND2	1:A:298:ASP:OD2	2.48	0.47
4:B:218:TYR:HB3	4:B:219:PRO:HD3	1.97	0.47
1:A:500:ALA:HB2	1:A:1294:PHE:HZ	1.80	0.46
1:A:628:MET:HG2	1:A:646:PHE:O	2.16	0.46
4:B:396:ARG:O	4:B:400:GLN:HG3	2.15	0.46
1:A:522:LEU:O	1:A:526:LEU:HD23	2.15	0.46
4:B:112:GLN:OE1	4:B:112:GLN:N	2.46	0.46
1:A:1637:ASN:HB2	1:A:1639:ARG:HG3	1.98	0.46
1:A:1308:PHE:CD2	1:A:1347:HIS:HA	2.51	0.46
1:A:1362:SER:HA	1:A:1404:PRO:HG3	1.98	0.46
9:A:2422:PT5:H18	9:A:2422:PT5:H52	1.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:280:LEU:HA	4:B:283:LEU:HD12	1.97	0.46
4:B:352:ALA:O	4:B:354:CYS:N	2.49	0.46
4:B:508:PRO:HG3	4:B:759:TYR:CD1	2.50	0.46
1:A:122:ASP:OD1	1:A:123:LYS:N	2.49	0.46
1:A:637:PHE:CE2	1:A:638:GLN:HG2	2.51	0.46
1:A:1289:TYR:CE1	1:A:1403:PHE:HD2	2.34	0.46
1:A:1818:ASP:O	1:A:1822:ARG:HD3	2.16	0.46
1:A:207:PRO:HA	1:A:210:GLN:HG3	1.97	0.46
4:B:50:THR:O	4:B:719:TYR:OH	2.29	0.46
4:B:193:PHE:HB3	4:B:218:TYR:CG	2.51	0.46
4:B:667:CYS:HA	4:B:697:CYS:HB2	1.98	0.46
1:A:1495:ALA:HB3	1:A:1500:GLU:HG3	1.97	0.45
1:A:126:MET:HA	1:A:129:ARG:HD2	1.98	0.45
3:D:236:GLY:HA3	3:D:245:THR:HG23	1.98	0.45
4:B:114:ARG:NH1	4:B:116:ASP:O	2.49	0.45
4:B:671:LYS:HA	4:B:671:LYS:HD3	1.82	0.45
1:A:1174:ARG:O	1:A:1180:ASN:ND2	2.48	0.45
1:A:1219:TRP:NE1	1:A:1269:LYS:HE2	2.32	0.45
1:A:120:ASP:OD2	4:B:265:SER:OG	2.18	0.45
1:A:1343:LYS:HD2	1:A:1347:HIS:CD2	2.52	0.45
4:B:828:THR:HG22	4:B:831:ARG:HH21	1.82	0.45
1:A:299:ASN:HB3	1:A:302:PHE:HD2	1.81	0.45
1:A:381:ILE:HG21	3:D:350:LYS:NZ	2.32	0.45
3:D:340:ILE:HD11	3:D:404:TYR:HE2	1.81	0.45
1:A:1367:TRP:CD1	1:A:1368:PRO:HD3	2.51	0.45
1:A:1483:LEU:HB3	1:A:1510:PHE:CZ	2.52	0.45
3:D:255:PHE:CD2	3:D:256:LEU:HD22	2.52	0.45
4:B:1031:LEU:HD23	4:B:1031:LEU:HA	1.86	0.45
1:A:201:LYS:HA	1:A:204:SER:HB3	1.99	0.45
1:A:336:PHE:O	1:A:340:ILE:HG12	2.17	0.45
1:A:1240:LYS:HG3	1:A:1242:LYS:H	1.82	0.45
4:B:1007:LYS:HA	4:B:1014:ILE:HA	1.99	0.45
1:A:146:GLY:O	1:A:150:ILE:HG12	2.17	0.44
1:A:1552:VAL:O	1:A:1556:ALA:N	2.49	0.44
4:B:735:VAL:HG22	4:B:741:THR:OG1	2.17	0.44
2:E:9:SER:HB3	2:E:12:MET:HG2	2.00	0.44
3:D:252:LEU:O	3:D:256:LEU:HD23	2.17	0.44
4:B:398:PRO:O	4:B:402:MET:HG3	2.17	0.44
1:A:1145:TYR:O	1:A:1148:THR:OG1	2.30	0.44
1:A:308:PHE:HE1	1:A:694:LEU:HD21	1.82	0.44
4:B:881:SER:OG	4:B:1026:CYS:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1580:ARG:O	1:A:1580:ARG:NE	2.47	0.44
4:B:157:ARG:NH2	4:B:222:PRO:O	2.49	0.44
4:B:753:GLN:NE2	4:B:785:PRO:HG2	2.33	0.44
1:A:1530:TYR:CE1	1:A:1536:ASN:HB3	2.52	0.44
4:B:569:ASP:O	4:B:573:GLU:HG3	2.17	0.44
4:B:1039:ASP:OD1	4:B:1040:GLY:N	2.51	0.44
4:B:470:THR:HG21	5:F:1:NAG:H5	2.00	0.44
1:A:124:THR:HG22	1:A:126:MET:H	1.82	0.44
4:B:660:PHE:HB2	4:B:741:THR:CG2	2.48	0.44
4:B:1001:ARG:HE	4:B:1020:SER:HB3	1.82	0.44
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.88	0.43
7:A:2403:R16:H361	7:A:2403:R16:H392	1.87	0.43
3:D:268:ARG:NH2	3:D:324:ASP:OD2	2.44	0.43
1:A:1539:ASP:O	1:A:1543:VAL:HG23	2.18	0.43
3:D:231:PRO:HA	3:D:319:VAL:HG23	1.99	0.43
1:A:1486:VAL:HG13	8:A:2412:Y01:HAC3	2.00	0.43
4:B:537:PRO:HD3	4:B:974:CYS:HB3	2.01	0.43
4:B:882:LEU:HD21	4:B:1016:ILE:HG21	2.00	0.43
1:A:108:ASN:HD21	1:A:198:ARG:HD3	1.83	0.43
1:A:1198:MET:O	1:A:1202:MET:HG2	2.19	0.43
8:A:2404:Y01:HAC2	8:A:2404:Y01:HAJ1	1.84	0.43
4:B:994:LEU:HD22	4:B:1001:ARG:HD3	2.00	0.43
1:A:311:ILE:O	1:A:344:SER:HB3	2.18	0.43
1:A:391:TRP:NE1	3:D:394:LEU:HA	2.34	0.43
3:D:264:ILE:HA	3:D:318:LEU:HB2	1.99	0.43
1:A:115:GLU:OE1	1:A:195:ARG:NH2	2.51	0.43
1:A:174:VAL:O	1:A:178:ILE:HG12	2.19	0.43
1:A:299:ASN:OD1	1:A:300:ILE:N	2.52	0.43
1:A:1248:LYS:O	1:A:1252:VAL:HG23	2.18	0.43
4:B:392:HIS:HE1	4:B:396:ARG:HE	1.67	0.43
4:B:780:PHE:CE1	4:B:870:GLN:HA	2.54	0.43
1:A:693:THR:O	1:A:697:ASN:HB2	2.18	0.43
1:A:1198:MET:HE1	1:A:1224:PHE:HD1	1.84	0.43
4:B:208:PHE:HD1	4:B:488:MET:SD	2.41	0.43
1:A:252:ALA:HB2	1:A:287:TRP:CE3	2.53	0.43
3:D:255:PHE:CZ	3:D:398:CYS:HB3	2.53	0.43
1:A:642:PRO:HA	2:E:12:MET:SD	2.59	0.43
1:A:1487:VAL:HG21	1:A:1510:PHE:HE2	1.84	0.43
1:A:1568:ARG:O	1:A:1571:ARG:HG2	2.19	0.43
4:B:261:SER:O	4:B:264:VAL:HG22	2.19	0.43
1:A:1259:LEU:O	1:A:1262:ILE:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:423:THR:CG2	4:B:426:TYR:HE2	2.28	0.42
1:A:1233:ALA:HB3	1:A:1251:ARG:HH21	1.85	0.42
1:A:1595:SER:OG	1:A:1710:ASN:ND2	2.45	0.42
3:D:303:GLN:HA	3:D:306:ILE:HD12	2.01	0.42
4:B:168:ILE:HG12	4:B:214:LEU:CD2	2.50	0.42
4:B:892:TYR:HA	4:B:982:PHE:O	2.19	0.42
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.81	0.42
1:A:1140:ARG:HD2	1:A:1203:ILE:HG21	2.00	0.42
3:D:265:SER:O	3:D:320:ALA:N	2.52	0.42
4:B:798:VAL:HG23	4:B:809:PRO:HD2	2.00	0.42
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.91	0.42
1:A:391:TRP:HE1	3:D:394:LEU:HA	1.84	0.42
1:A:1632:ILE:HD11	1:A:1664:CYS:SG	2.59	0.42
4:B:646:GLU:HA	4:B:649:LYS:HZ3	1.85	0.42
1:A:1215:PHE:HD1	1:A:1221:ILE:HG13	1.85	0.42
8:A:2421:Y01:HAJ2	8:A:2421:Y01:HAB2	1.78	0.42
2:E:17:THR:O	2:E:17:THR:HG22	2.19	0.42
3:D:232:ILE:HA	3:D:340:ILE:CG2	2.48	0.42
3:D:266:ILE:HA	3:D:320:ALA:HB3	2.00	0.42
3:D:343:TYR:HB2	3:D:385:PHE:CD1	2.54	0.42
4:B:258:VAL:HG12	4:B:260:VAL:HG13	2.01	0.42
4:B:596:ASP:OD1	4:B:596:ASP:N	2.50	0.42
1:A:275:ARG:NH2	1:A:1634:ARG:HD3	2.35	0.42
4:B:52:SER:OG	4:B:814:ILE:HG12	2.20	0.42
1:A:1546:SER:O	1:A:1550:ILE:HG12	2.19	0.42
1:A:1731:ARG:HD2	1:A:1731:ARG:HA	1.91	0.42
1:A:1732:VAL:HG21	1:A:1752:MET:HG3	2.02	0.42
4:B:37:VAL:HA	4:B:40:MET:HG2	2.01	0.42
4:B:306:HIS:CG	4:B:349:VAL:HG11	2.54	0.42
1:A:369:ARG:HD2	1:A:369:ARG:HA	1.90	0.42
1:A:1465:TRP:O	1:A:1469:VAL:HG23	2.20	0.42
4:B:752:TRP:NE1	4:B:754:GLU:HB2	2.35	0.42
1:A:1309:PHE:O	1:A:1384:PRO:HD3	2.20	0.41
1:A:1331:LYS:C	1:A:1333:GLU:H	2.24	0.41
8:A:2404:Y01:HAJ1	8:A:2404:Y01:HAA3	1.71	0.41
4:B:224:VAL:HG23	4:B:225:ASP:N	2.30	0.41
4:B:645:SER:HB3	4:B:687:ILE:HG21	2.02	0.41
1:A:237:PHE:CG	1:A:339:LEU:HD13	2.55	0.41
1:A:1313:ASP:HB3	1:A:1326:TYR:CD2	2.55	0.41
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.93	0.41
1:A:737:LYS:HE2	1:A:737:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:432:ARG:HB2	4:B:433:PRO:HD3	2.01	0.41
4:B:689:ARG:O	4:B:689:ARG:HG2	2.21	0.41
1:A:299:ASN:HD21	8:A:2412:Y01:CAZ	2.34	0.41
1:A:1457:ARG:NH2	1:A:1462:TYR:OH	2.53	0.41
1:A:1686:PHE:CE2	7:A:2401:R16:H282	2.56	0.41
7:A:2401:R16:H322	7:A:2401:R16:H292	1.94	0.41
4:B:100:LEU:HB3	4:B:488:MET:CE	2.50	0.41
3:D:392:ASN:OD1	3:D:393:GLN:HG2	2.21	0.41
3:D:405:LEU:HD23	3:D:405:LEU:HA	1.87	0.41
4:B:396:ARG:HD3	4:B:410:TYR:OH	2.21	0.41
4:B:860:LEU:HD22	4:B:1013:LEU:HD21	2.02	0.41
1:A:382:GLU:OE2	3:D:354:ARG:NH2	2.54	0.41
8:A:2404:Y01:HAA1	8:A:2404:Y01:HAP2	2.02	0.41
8:A:2404:Y01:HAS2	8:A:2404:Y01:HAE1	1.88	0.41
1:A:143:PHE:CZ	1:A:147:ILE:HD11	2.56	0.41
1:A:254:PHE:HB2	1:A:284:ARG:HG3	2.03	0.41
1:A:389:LEU:HD12	1:A:543:ARG:HH12	1.86	0.41
1:A:1497:TYR:HA	1:A:1500:GLU:HB2	2.02	0.41
4:B:1005:GLY:HA2	4:B:1015:PHE:O	2.20	0.41
1:A:311:ILE:HD12	1:A:343:GLY:HA3	2.03	0.41
1:A:712:LEU:HD12	1:A:1413:ALA:HB3	2.02	0.41
1:A:1367:TRP:N	1:A:1368:PRO:HD2	2.36	0.41
1:A:1726:LEU:HD22	1:A:1795:LEU:HD22	2.03	0.41
3:D:228:SER:OG	3:D:313:ALA:O	2.20	0.41
4:B:146:LYS:HA	4:B:147:PRO:HD3	1.93	0.41
4:B:289:VAL:HG12	4:B:310:ALA:HB2	2.03	0.41
4:B:472:GLN:O	4:B:473:PHE:HB2	2.21	0.41
4:B:653:PHE:CZ	4:B:659:THR:HB	2.56	0.41
4:B:991:SER:HB3	4:B:1004:HIS:ND1	2.35	0.41
1:A:525:PHE:CD2	1:A:578:ARG:HD2	2.56	0.41
4:B:33:ILE:HA	4:B:36:TRP:HB3	2.02	0.41
4:B:856:GLY:HA2	4:B:981:TYR:HB2	2.02	0.41
1:A:1218:LEU:HB2	7:A:2420:R16:H281	2.02	0.40
1:A:1756:MET:SD	1:A:1757:SER:N	2.94	0.40
4:B:241:ARG:O	4:B:245:ILE:HG12	2.21	0.40
4:B:421:ILE:O	4:B:425:GLU:HG3	2.21	0.40
1:A:331:TRP:HE3	1:A:334:LEU:HD12	1.86	0.40
1:A:1194:PHE:HE2	1:A:1257:ARG:HD3	1.86	0.40
1:A:1304:PHE:CE1	1:A:1392:LEU:HD13	2.55	0.40
1:A:1474:GLU:O	1:A:1477:ILE:HG22	2.22	0.40
1:A:1487:VAL:HA	1:A:1490:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1730:ILE:HD13	1:A:1730:ILE:HA	1.97	0.40
8:A:2421:Y01:HAP2	8:A:2421:Y01:HAO1	1.97	0.40
4:B:93:ARG:HB2	4:B:446:TRP:HH2	1.85	0.40
4:B:766:ARG:NH2	4:B:855:ASP:HB2	2.36	0.40
1:A:235:LEU:HD11	1:A:1489:MET:SD	2.61	0.40
1:A:277:CYS:HB3	1:A:281:THR:OG1	2.22	0.40
4:B:193:PHE:CG	4:B:218:TYR:HB2	2.55	0.40
4:B:258:VAL:HG13	4:B:272:ILE:HG21	2.04	0.40
4:B:735:VAL:HB	4:B:811:VAL:HG12	2.02	0.40
1:A:92:THR:O	1:A:94:TRP:HD1	2.04	0.40
1:A:157:HIS:C	1:A:159:GLY:H	2.24	0.40
1:A:242:LEU:HD12	1:A:300:ILE:HD13	2.03	0.40
1:A:724:GLU:O	1:A:727:GLU:HG3	2.21	0.40
1:A:1465:TRP:CE2	1:A:1469:VAL:HG21	2.56	0.40
1:A:1675:ASN:OD1	1:A:1675:ASN:N	2.55	0.40
4:B:780:PHE:HE1	4:B:870:GLN:HA	1.86	0.40
1:A:262:PRO:HG3	1:A:287:TRP:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1248/2339 (53%)	1199 (96%)	49 (4%)	0	100	100
2	E	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
3	D	159/598 (27%)	154 (97%)	5 (3%)	0	100	100
4	B	947/1103 (86%)	898 (95%)	49 (5%)	0	100	100
All	All	2377/4065 (58%)	2271 (96%)	106 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1089/1991 (55%)	1087 (100%)	2 (0%)	92	97
2	E	20/20 (100%)	20 (100%)	0	100	100
3	D	135/510 (26%)	135 (100%)	0	100	100
4	B	846/971 (87%)	843 (100%)	3 (0%)	89	95
All	All	2090/3492 (60%)	2085 (100%)	5 (0%)	91	97

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

Mol	Chain	Res	Type
1	A	546	PHE
1	A	1484	ASN
4	B	689	ARG
4	B	722	LYS
4	B	1053	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	1435	ASN
4	B	392	HIS
4	B	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1	5,4	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	C	2	5	14,14,15	0.20	0	17,19,21	0.44	0
5	BMA	C	3	5	11,11,12	0.60	0	15,15,17	0.75	0
5	NAG	F	1	5,4	14,14,15	0.42	0	17,19,21	0.48	0
5	NAG	F	2	5	14,14,15	0.18	0	17,19,21	0.53	0
5	BMA	F	3	5	11,11,12	0.58	0	15,15,17	0.69	0
6	NAG	G	1	4,6	14,14,15	0.79	1 (7%)	17,19,21	1.00	1 (5%)
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.45	0
6	BMA	G	3	6	11,11,12	0.64	0	15,15,17	0.80	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	C	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
6	NAG	G	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	BMA	G	3	6	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1	NAG	O5-C1	2.71	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	1	NAG	C1-O5-C5	3.85	117.40	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

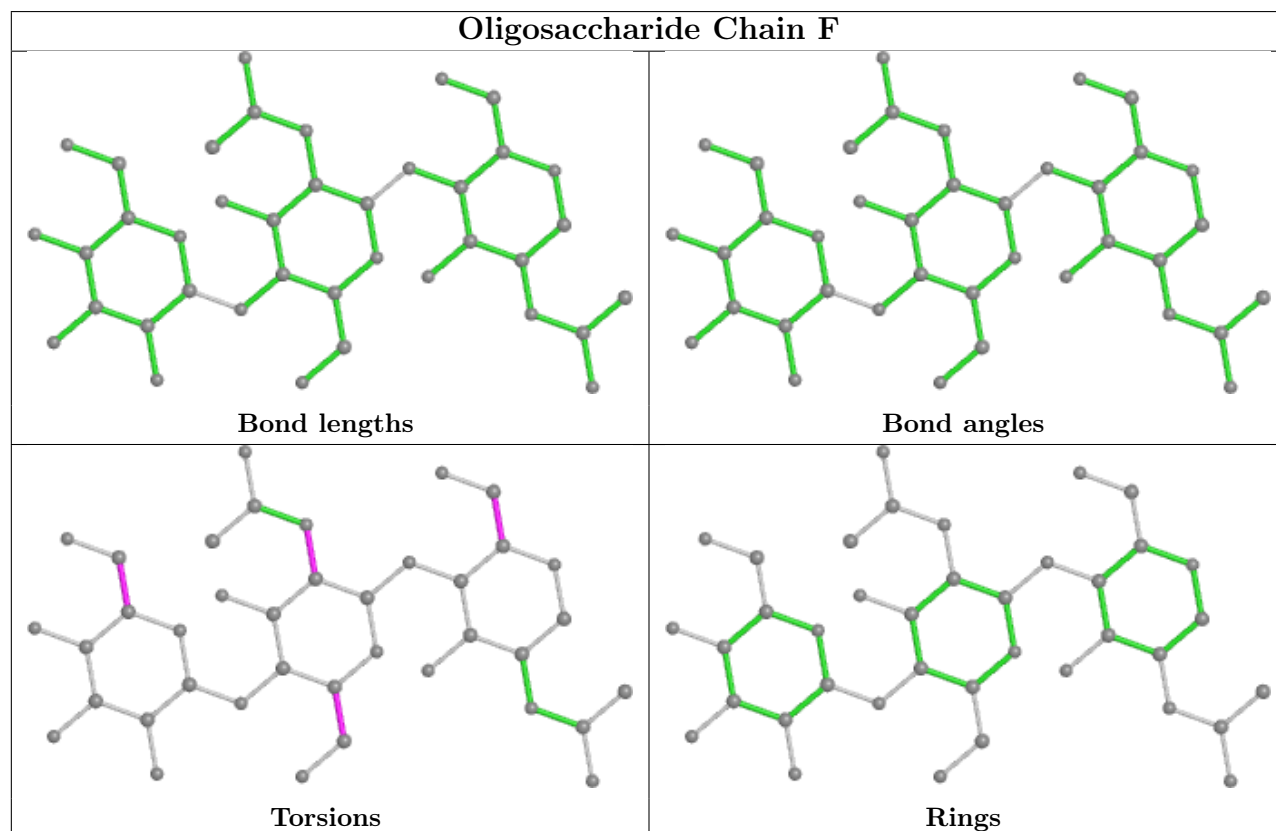
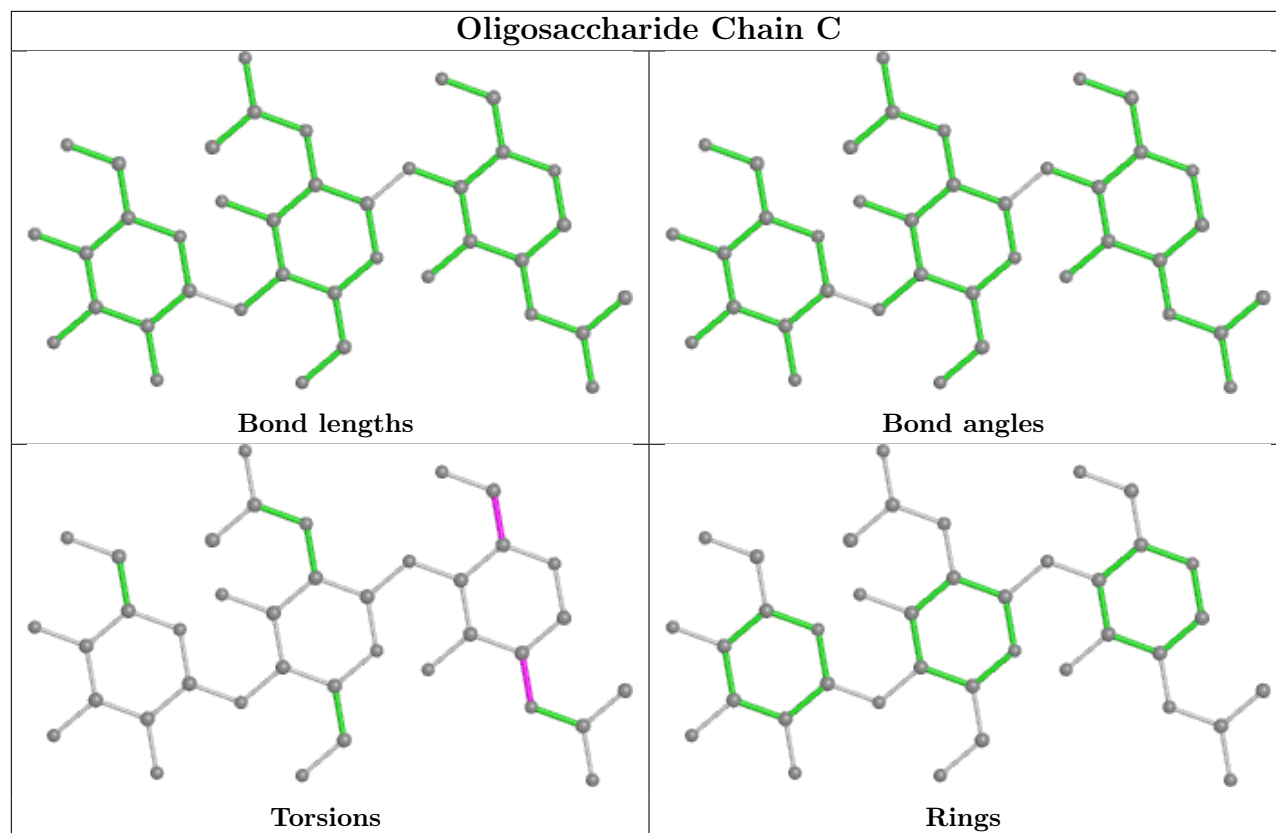
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
6	G	3	BMA	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C3-C2-N2-C7
5	C	1	NAG	C3-C2-N2-C7

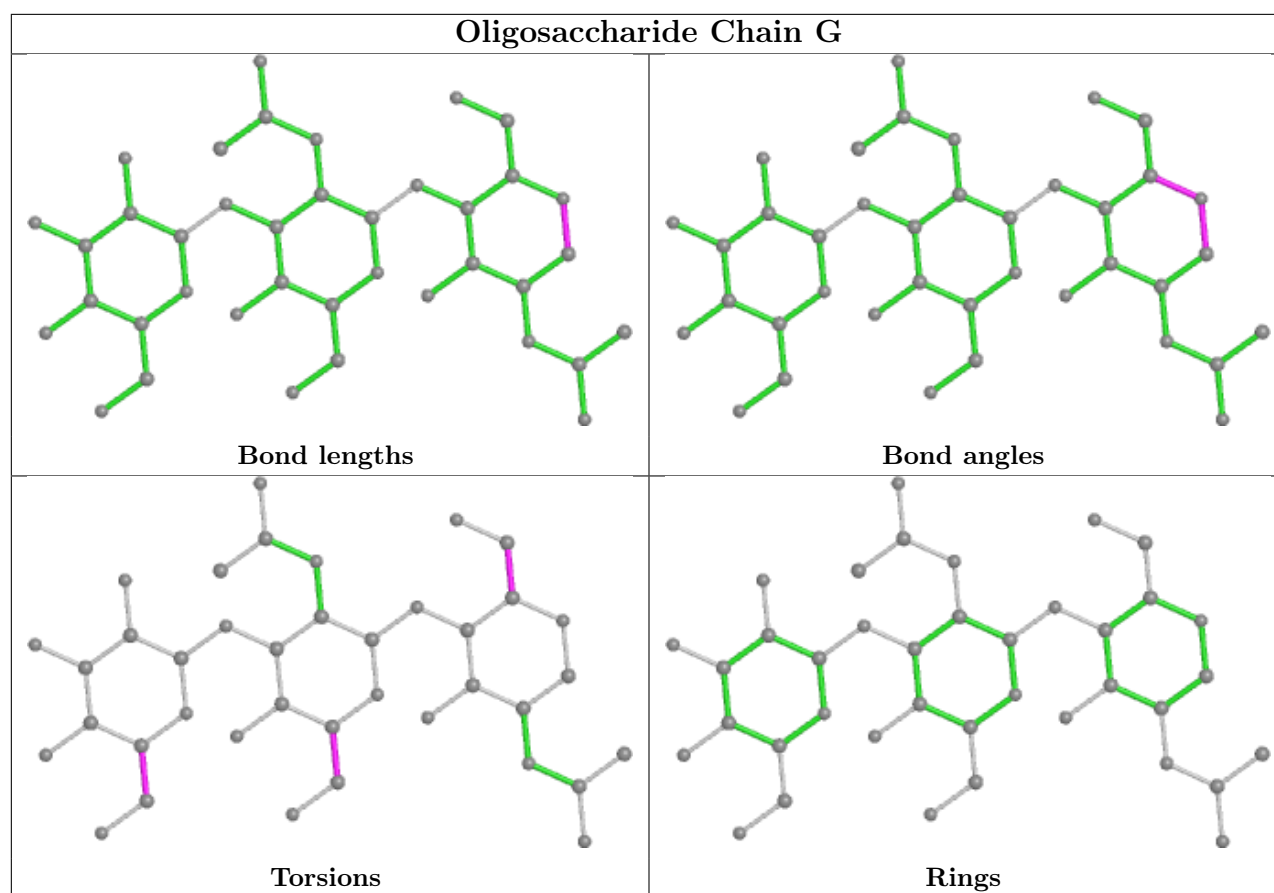
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	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.





5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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	$\# Z > 2$
11	NAG	B	1202	4	14,14,15	0.25	0	17,19,21	0.44	0
8	Y01	A	2412	-	38,38,38	3.97	12 (31%)	57,57,57	2.14	19 (33%)
7	R16	A	2410	-	15,15,15	0.10	0	14,14,14	0.15	0
7	R16	A	2411	-	10,10,15	0.09	0	9,9,14	0.17	0
11	NAG	B	1203	4	14,14,15	0.23	0	17,19,21	0.55	0
7	R16	A	2407	-	15,15,15	0.10	0	14,14,14	0.18	0
7	R16	A	2414	-	14,14,15	0.10	0	13,13,14	0.20	0
11	NAG	B	1205	4	14,14,15	0.18	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	B	1204	4	14,14,15	0.34	0	17,19,21	0.49	0
7	R16	A	2406	-	15,15,15	0.10	0	14,14,14	0.19	0
11	NAG	B	1207	4	14,14,15	0.24	0	17,19,21	0.54	0
8	Y01	A	2421	-	38,38,38	4.02	12 (31%)	57,57,57	2.09	16 (28%)
7	R16	A	2403	-	15,15,15	0.10	0	14,14,14	0.14	0
7	R16	A	2409	-	15,15,15	0.09	0	14,14,14	0.13	0
7	R16	A	2413	-	12,12,15	0.09	0	11,11,14	0.14	0
7	R16	A	2416	-	11,11,15	0.09	0	10,10,14	0.17	0
8	Y01	A	2404	-	38,38,38	4.01	12 (31%)	57,57,57	2.08	16 (28%)
7	R16	A	2420	-	15,15,15	0.10	0	14,14,14	0.18	0
7	R16	A	2405	-	15,15,15	0.10	0	14,14,14	0.18	0
9	PT5	A	2422	-	61,61,69	0.50	0	75,79,87	0.74	3 (4%)
7	R16	A	2408	-	15,15,15	0.12	0	14,14,14	0.20	0
7	R16	A	2402	-	15,15,15	0.12	0	14,14,14	0.15	0
7	R16	A	2417	-	14,14,15	0.10	0	13,13,14	0.30	0
7	R16	A	2401	-	15,15,15	0.10	0	14,14,14	0.17	0
11	NAG	B	1206	4	14,14,15	0.20	0	17,19,21	0.40	0
7	R16	A	2418	-	12,12,15	0.10	0	11,11,14	0.18	0
11	NAG	B	1201	4	14,14,15	0.22	0	17,19,21	0.48	0
11	NAG	B	1208	4	14,14,15	0.22	0	17,19,21	0.50	0
7	R16	A	2419	-	15,15,15	0.11	0	14,14,14	0.17	0
7	R16	A	2415	-	12,12,15	0.10	0	11,11,14	0.18	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
11	NAG	B	1202	4	-	0/6/23/26	0/1/1/1
8	Y01	A	2412	-	-	8/19/77/77	0/4/4/4
7	R16	A	2410	-	-	8/13/13/13	-
7	R16	A	2411	-	-	3/8/8/13	-
11	NAG	B	1203	4	-	3/6/23/26	0/1/1/1
7	R16	A	2407	-	-	1/13/13/13	-
7	R16	A	2414	-	-	5/12/12/13	-
11	NAG	B	1205	4	-	2/6/23/26	0/1/1/1
11	NAG	B	1204	4	-	3/6/23/26	0/1/1/1
7	R16	A	2406	-	-	5/13/13/13	-
11	NAG	B	1207	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	Y01	A	2421	-	-	14/19/77/77	0/4/4/4
7	R16	A	2403	-	-	8/13/13/13	-
7	R16	A	2409	-	-	3/13/13/13	-
7	R16	A	2413	-	-	2/10/10/13	-
7	R16	A	2416	-	-	3/9/9/13	-
8	Y01	A	2404	-	-	14/19/77/77	0/4/4/4
7	R16	A	2420	-	-	5/13/13/13	-
7	R16	A	2405	-	-	7/13/13/13	-
9	PT5	A	2422	-	-	27/58/82/90	0/1/1/1
7	R16	A	2408	-	-	8/13/13/13	-
7	R16	A	2402	-	-	5/13/13/13	-
7	R16	A	2417	-	-	6/12/12/13	-
7	R16	A	2401	-	-	4/13/13/13	-
11	NAG	B	1206	4	-	0/6/23/26	0/1/1/1
7	R16	A	2418	-	-	3/10/10/13	-
11	NAG	B	1201	4	-	2/6/23/26	0/1/1/1
11	NAG	B	1208	4	-	0/6/23/26	0/1/1/1
7	R16	A	2419	-	-	2/13/13/13	-
7	R16	A	2415	-	-	2/10/10/13	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2404	Y01	CAI-CAZ	16.40	1.69	1.33
8	A	2421	Y01	CAI-CAZ	16.39	1.69	1.33
8	A	2412	Y01	CAI-CAZ	16.29	1.68	1.33
8	A	2404	Y01	CAU-CBI	-7.08	1.41	1.54
8	A	2404	Y01	CBH-CBF	6.97	1.67	1.56
8	A	2421	Y01	CAQ-CAP	6.95	1.73	1.54
8	A	2404	Y01	CAQ-CAP	6.89	1.72	1.54
8	A	2421	Y01	CBH-CBF	6.89	1.67	1.56
8	A	2421	Y01	CAU-CBI	-6.87	1.41	1.54
8	A	2412	Y01	CBH-CBF	6.82	1.67	1.56
8	A	2412	Y01	CAQ-CAP	6.74	1.72	1.54
8	A	2412	Y01	CAU-CBI	-6.72	1.42	1.54
8	A	2421	Y01	CAK-CBD	6.23	1.63	1.53
8	A	2404	Y01	CAK-CBD	6.17	1.63	1.53
8	A	2412	Y01	CAU-CAS	6.05	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2421	Y01	CAU-CAS	5.97	1.66	1.53
8	A	2412	Y01	CAK-CBD	5.88	1.63	1.53
8	A	2404	Y01	CAU-CAS	5.86	1.65	1.53
8	A	2412	Y01	CBI-CBE	5.67	1.65	1.55
8	A	2421	Y01	CBI-CBE	5.62	1.65	1.55
8	A	2404	Y01	CBI-CBE	5.52	1.65	1.55
8	A	2421	Y01	CAQ-CBG	5.13	1.65	1.54
8	A	2404	Y01	CAQ-CBG	5.09	1.64	1.54
8	A	2412	Y01	CBB-CBE	-5.08	1.45	1.54
8	A	2412	Y01	CAQ-CBG	5.00	1.64	1.54
8	A	2421	Y01	CBB-CBE	-4.97	1.45	1.54
8	A	2404	Y01	CBB-CBE	-4.76	1.46	1.54
8	A	2421	Y01	OAW-CAY	3.19	1.43	1.34
8	A	2404	Y01	OAW-CAY	3.10	1.43	1.34
8	A	2412	Y01	OAW-CAY	3.02	1.42	1.34
8	A	2404	Y01	CAO-CBB	2.97	1.62	1.54
8	A	2421	Y01	CAO-CBB	2.77	1.61	1.54
8	A	2412	Y01	CAO-CBB	2.68	1.61	1.54
8	A	2412	Y01	CBH-CAZ	-2.43	1.48	1.52
8	A	2421	Y01	CBH-CAZ	-2.40	1.48	1.52
8	A	2404	Y01	CBH-CAZ	-2.17	1.48	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2404	Y01	CAD-CBH-CBF	-5.86	104.70	111.68
8	A	2412	Y01	CAK-CAI-CAZ	-5.41	115.08	125.06
8	A	2412	Y01	CAU-CBI-CBE	5.13	124.25	116.57
8	A	2421	Y01	CAU-CBI-CBE	5.02	124.09	116.57
8	A	2421	Y01	CAD-CBH-CBF	-4.82	105.93	111.68
8	A	2412	Y01	CAD-CBH-CBF	-4.80	105.96	111.68
8	A	2421	Y01	CBH-CAZ-CAI	-4.72	115.67	122.90
8	A	2412	Y01	CBG-CBI-CBE	4.49	105.39	100.07
8	A	2421	Y01	OAW-CAY-CAM	4.43	121.04	111.50
8	A	2404	Y01	OAW-CAY-CAM	4.34	120.85	111.50
8	A	2421	Y01	CAK-CAI-CAZ	-4.28	117.16	125.06
8	A	2404	Y01	CAU-CBI-CBE	4.27	122.96	116.57
8	A	2404	Y01	CAK-CAI-CAZ	-4.25	117.23	125.06
8	A	2412	Y01	OAW-CAY-CAM	4.20	120.55	111.50
8	A	2412	Y01	CBH-CAZ-CAI	-4.17	116.52	122.90
8	A	2412	Y01	CAE-CBI-CBG	-3.98	104.29	111.71
8	A	2404	Y01	CBG-CBI-CBE	3.87	104.66	100.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2421	Y01	CAU-CBI-CBG	3.78	113.14	107.27
8	A	2404	Y01	CAE-CBI-CBG	-3.65	104.91	111.71
8	A	2421	Y01	CBC-CAV-CAZ	3.46	116.90	111.52
8	A	2404	Y01	CBH-CAZ-CAI	-3.45	117.62	122.90
8	A	2412	Y01	CAE-CBI-CBE	-3.37	105.42	111.71
8	A	2421	Y01	CAE-CBI-CAU	-3.33	105.34	110.59
8	A	2404	Y01	CAE-CBI-CAU	-3.25	105.46	110.59
8	A	2404	Y01	CBI-CBE-CBB	-3.19	114.50	119.49
8	A	2421	Y01	CAE-CBI-CBE	-3.16	105.82	111.71
8	A	2421	Y01	CAE-CBI-CBG	-3.15	105.84	111.71
8	A	2421	Y01	CBF-CBD-CBG	3.12	113.27	109.09
8	A	2404	Y01	CAE-CBI-CBE	-3.12	105.89	111.71
8	A	2421	Y01	CAC-CBB-CBE	-3.10	108.18	112.92
8	A	2404	Y01	CBF-CBH-CAZ	2.98	114.33	109.65
8	A	2404	Y01	CAO-CBB-CBE	2.94	116.37	110.28
8	A	2412	Y01	CAE-CBI-CAU	-2.87	106.06	110.59
8	A	2404	Y01	CAC-CBB-CBE	-2.78	108.66	112.92
8	A	2404	Y01	CAU-CBI-CBG	2.76	111.55	107.27
8	A	2412	Y01	CAK-CBD-CBF	2.63	112.90	109.71
9	A	2422	PT5	C3-C2-C1	2.59	115.58	109.68
8	A	2412	Y01	CBI-CBG-CBD	-2.53	110.64	114.38
8	A	2412	Y01	CBF-CBH-CAZ	2.35	113.34	109.65
8	A	2421	Y01	CAC-CBB-CAO	-2.34	106.69	110.36
8	A	2412	Y01	CAP-CBE-CBB	-2.34	108.52	112.15
8	A	2412	Y01	CBI-CBE-CBB	-2.34	115.83	119.49
8	A	2421	Y01	CAT-CAR-CBC	2.33	114.30	110.33
8	A	2404	Y01	CAS-CBF-CBH	-2.30	110.06	113.08
8	A	2421	Y01	CAO-CBB-CBE	2.23	114.90	110.28
8	A	2412	Y01	CAQ-CBG-CBI	2.20	106.49	103.84
8	A	2412	Y01	CAL-CAM-CAY	-2.19	107.07	113.43
8	A	2412	Y01	CAC-CBB-CAO	-2.15	107.00	110.36
9	A	2422	PT5	O16-C10-C12	2.09	116.01	111.50
8	A	2421	Y01	CAL-CAM-CAY	-2.08	107.38	113.43
8	A	2404	Y01	CAQ-CBG-CBD	2.08	122.50	119.08
8	A	2412	Y01	CAQ-CBG-CBD	2.08	122.50	119.08
8	A	2412	Y01	CAT-CAR-CBC	2.04	113.81	110.33
9	A	2422	PT5	C6-C5-C4	-2.04	107.01	111.66

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2404	Y01	CAO-CBB-CBE-CAP
8	A	2404	Y01	CAC-CBB-CBE-CAP
8	A	2421	Y01	CAV-CBC-OAW-CAY
8	A	2421	Y01	CAM-CAY-OAW-CBC
9	A	2422	PT5	C5-O5-P5-O53
9	A	2422	PT5	O19-C11-O18-C9
9	A	2422	PT5	C31-C11-O18-C9
9	A	2422	PT5	C22-C23-C24-C25
8	A	2421	Y01	CAC-CBB-CBE-CBI
8	A	2404	Y01	CAO-CBB-CBE-CBI
8	A	2421	Y01	OAG-CAY-OAW-CBC
8	A	2404	Y01	CAJ-CAO-CBB-CAC
11	B	1207	NAG	O5-C5-C6-O6
8	A	2404	Y01	CAC-CBB-CBE-CBI
8	A	2421	Y01	CAO-CBB-CBE-CBI
9	A	2422	PT5	C14-C15-C16-C17
8	A	2421	Y01	CAC-CBB-CBE-CAP
11	B	1205	NAG	O5-C5-C6-O6
11	B	1201	NAG	O5-C5-C6-O6
11	B	1204	NAG	O5-C5-C6-O6
11	B	1207	NAG	C4-C5-C6-O6
11	B	1203	NAG	O5-C5-C6-O6
7	A	2406	R16	C30-C31-C32-C33
11	B	1204	NAG	C4-C5-C6-O6
11	B	1201	NAG	C4-C5-C6-O6
8	A	2412	Y01	CAJ-CAO-CBB-CBE
8	A	2421	Y01	CAJ-CAO-CBB-CBE
11	B	1203	NAG	C4-C5-C6-O6
7	A	2420	R16	C35-C36-C37-C38
11	B	1205	NAG	C4-C5-C6-O6
8	A	2421	Y01	CAO-CAJ-CAN-CBA
8	A	2412	Y01	CAJ-CAO-CBB-CAC
8	A	2404	Y01	CAJ-CAO-CBB-CBE
8	A	2421	Y01	CAJ-CAO-CBB-CAC
8	A	2404	Y01	CAO-CAJ-CAN-CBA
9	A	2422	PT5	C12-C10-O16-C8
9	A	2422	PT5	O17-C10-O16-C8
7	A	2415	R16	C36-C37-C38-C39
7	A	2402	R16	C28-C29-C30-C31
7	A	2405	R16	C34-C35-C36-C37
7	A	2408	R16	C28-C29-C30-C31
7	A	2403	R16	C32-C33-C34-C35
7	A	2405	R16	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
7	A	2410	R16	C29-C30-C31-C32
7	A	2401	R16	C28-C29-C30-C31
7	A	2402	R16	C36-C37-C38-C39
7	A	2413	R16	C33-C34-C35-C36
7	A	2417	R16	C28-C29-C30-C31
9	A	2422	PT5	C31-C32-C33-C34
9	A	2422	PT5	C26-C27-C28-C29
7	A	2401	R16	C29-C30-C31-C32
7	A	2414	R16	C29-C30-C31-C32
7	A	2405	R16	C36-C37-C38-C39
9	A	2422	PT5	C25-C26-C27-C28
7	A	2409	R16	C34-C35-C36-C37
7	A	2420	R16	C28-C29-C30-C31
9	A	2422	PT5	C34-C35-C36-C37
7	A	2408	R16	C33-C34-C35-C36
7	A	2405	R16	C29-C30-C31-C32
7	A	2418	R16	C32-C33-C34-C35
7	A	2403	R16	C34-C35-C36-C37
7	A	2417	R16	C32-C33-C34-C35
7	A	2410	R16	C35-C36-C37-C38
9	A	2422	PT5	C36-C37-C38-C39
7	A	2410	R16	C33-C34-C35-C36
9	A	2422	PT5	C10-C12-C13-C14
9	A	2422	PT5	C27-C28-C29-C30
7	A	2408	R16	C29-C30-C31-C32
7	A	2408	R16	C34-C35-C36-C37
7	A	2415	R16	C33-C34-C35-C36
9	A	2422	PT5	C24-C25-C26-C27
8	A	2421	Y01	CAO-CBB-CBE-CAP
9	A	2422	PT5	C33-C34-C35-C36
7	A	2414	R16	C33-C34-C35-C36
7	A	2403	R16	C35-C36-C37-C38
7	A	2402	R16	C37-C38-C39-C40
7	A	2403	R16	C33-C34-C35-C36
7	A	2408	R16	C39-C40-C41-C42
7	A	2405	R16	C39-C40-C41-C42
7	A	2403	R16	C29-C30-C31-C32
7	A	2411	R16	C34-C35-C36-C37
7	A	2401	R16	C36-C37-C38-C39
9	A	2422	PT5	C32-C33-C34-C35
7	A	2419	R16	C34-C35-C36-C37
7	A	2419	R16	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
7	A	2416	R16	C32-C33-C34-C35
7	A	2408	R16	C38-C39-C40-C41
7	A	2410	R16	C34-C35-C36-C37
7	A	2402	R16	C27-C28-C29-C30
7	A	2405	R16	C32-C33-C34-C35
7	A	2417	R16	C35-C36-C37-C38
9	A	2422	PT5	C19-C20-C21-C22
9	A	2422	PT5	C21-C22-C23-C24
7	A	2402	R16	C35-C36-C37-C38
7	A	2410	R16	C32-C33-C34-C35
9	A	2422	PT5	C5-O5-P5-O52
8	A	2404	Y01	CAN-CAJ-CAO-CBB
7	A	2417	R16	C31-C32-C33-C34
7	A	2411	R16	C35-C36-C37-C38
7	A	2417	R16	C36-C37-C38-C39
7	A	2403	R16	C39-C40-C41-C42
7	A	2406	R16	C33-C34-C35-C36
8	A	2404	Y01	CAJ-CAN-CBA-CAA
7	A	2406	R16	C35-C36-C37-C38
7	A	2414	R16	C36-C37-C38-C39
8	A	2421	Y01	CAJ-CAN-CBA-CAB
7	A	2420	R16	C29-C30-C31-C32
7	A	2408	R16	C35-C36-C37-C38
7	A	2413	R16	C31-C32-C33-C34
7	A	2416	R16	C31-C32-C33-C34
8	A	2412	Y01	CAJ-CAN-CBA-CAB
7	A	2410	R16	C39-C40-C41-C42
9	A	2422	PT5	C9-C8-O16-C10
9	A	2422	PT5	C11-C31-C32-C33
9	A	2422	PT5	C7-O13-P1-O1
7	A	2410	R16	C38-C39-C40-C41
11	B	1207	NAG	C3-C2-N2-C7
9	A	2422	PT5	C20-C21-C22-C23
7	A	2410	R16	C36-C37-C38-C39
7	A	2417	R16	C37-C38-C39-C40
7	A	2414	R16	C30-C31-C32-C33
7	A	2420	R16	C36-C37-C38-C39
11	B	1204	NAG	C1-C2-N2-C7
7	A	2408	R16	C32-C33-C34-C35
7	A	2418	R16	C33-C34-C35-C36
8	A	2404	Y01	CAJ-CAN-CBA-CAB
9	A	2422	PT5	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
7	A	2418	R16	C37-C38-C39-C40
7	A	2414	R16	C31-C32-C33-C34
7	A	2409	R16	C31-C32-C33-C34
7	A	2406	R16	C28-C29-C30-C31
8	A	2421	Y01	CAM-CAL-CAX-OAH
7	A	2406	R16	C31-C32-C33-C34
7	A	2401	R16	C27-C28-C29-C30
8	A	2404	Y01	CAM-CAL-CAX-OAF
7	A	2420	R16	C38-C39-C40-C41
8	A	2404	Y01	CAM-CAL-CAX-OAH
8	A	2421	Y01	CAJ-CAN-CBA-CAA
7	A	2411	R16	C36-C37-C38-C39
9	A	2422	PT5	C13-C14-C15-C16
8	A	2412	Y01	CAX-CAL-CAM-CAY
8	A	2421	Y01	CAM-CAL-CAX-OAF
8	A	2412	Y01	CAM-CAL-CAX-OAH
8	A	2412	Y01	CAM-CAL-CAX-OAF
8	A	2404	Y01	CAL-CAM-CAY-OAW
11	B	1203	NAG	C3-C2-N2-C7
7	A	2403	R16	C28-C29-C30-C31
7	A	2403	R16	C36-C37-C38-C39
7	A	2416	R16	C37-C38-C39-C40
8	A	2404	Y01	CAL-CAM-CAY-OAG
9	A	2422	PT5	C7-C8-O16-C10
7	A	2407	R16	C30-C31-C32-C33
8	A	2412	Y01	OAG-CAY-OAW-CBC
7	A	2405	R16	C35-C36-C37-C38
8	A	2412	Y01	CAJ-CAN-CBA-CAA
7	A	2409	R16	C33-C34-C35-C36

There are no ring outliers.

15 monomers are involved in 27 short contacts:

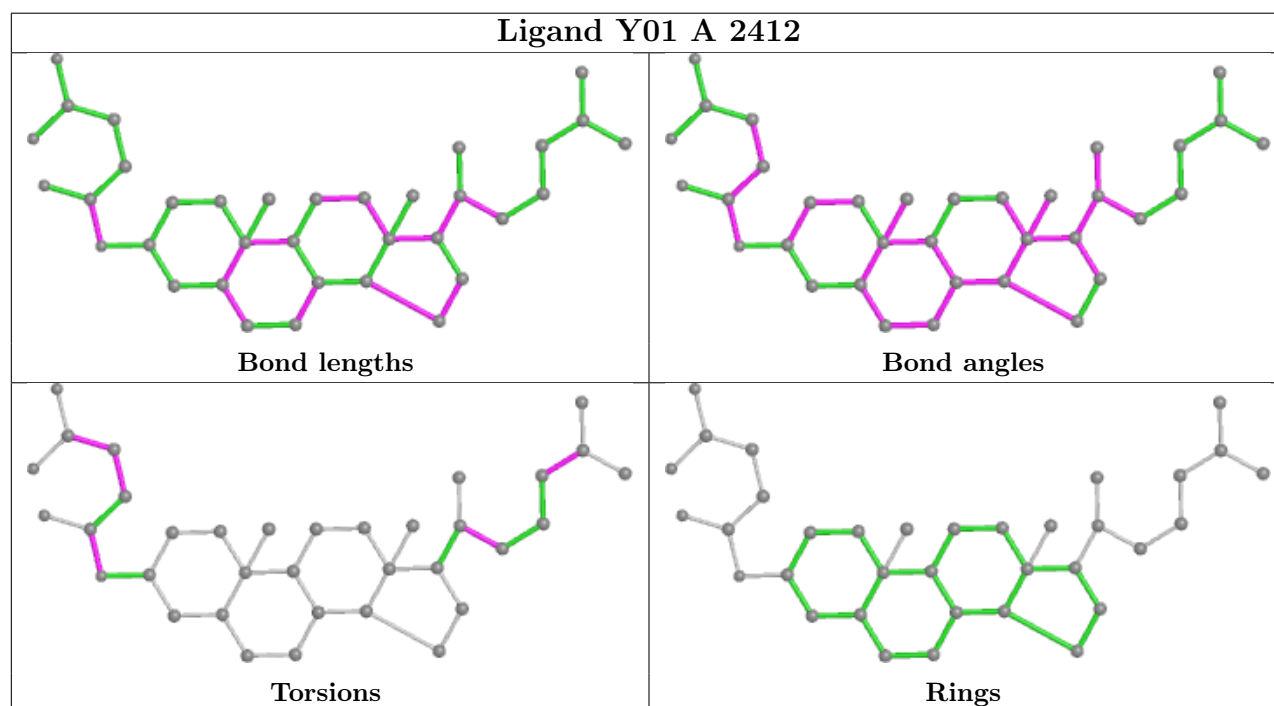
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2412	Y01	3	0
7	A	2410	R16	1	0
7	A	2407	R16	1	0
7	A	2414	R16	1	0
11	B	1205	NAG	1	0
11	B	1204	NAG	1	0
8	A	2421	Y01	2	0
7	A	2403	R16	2	0

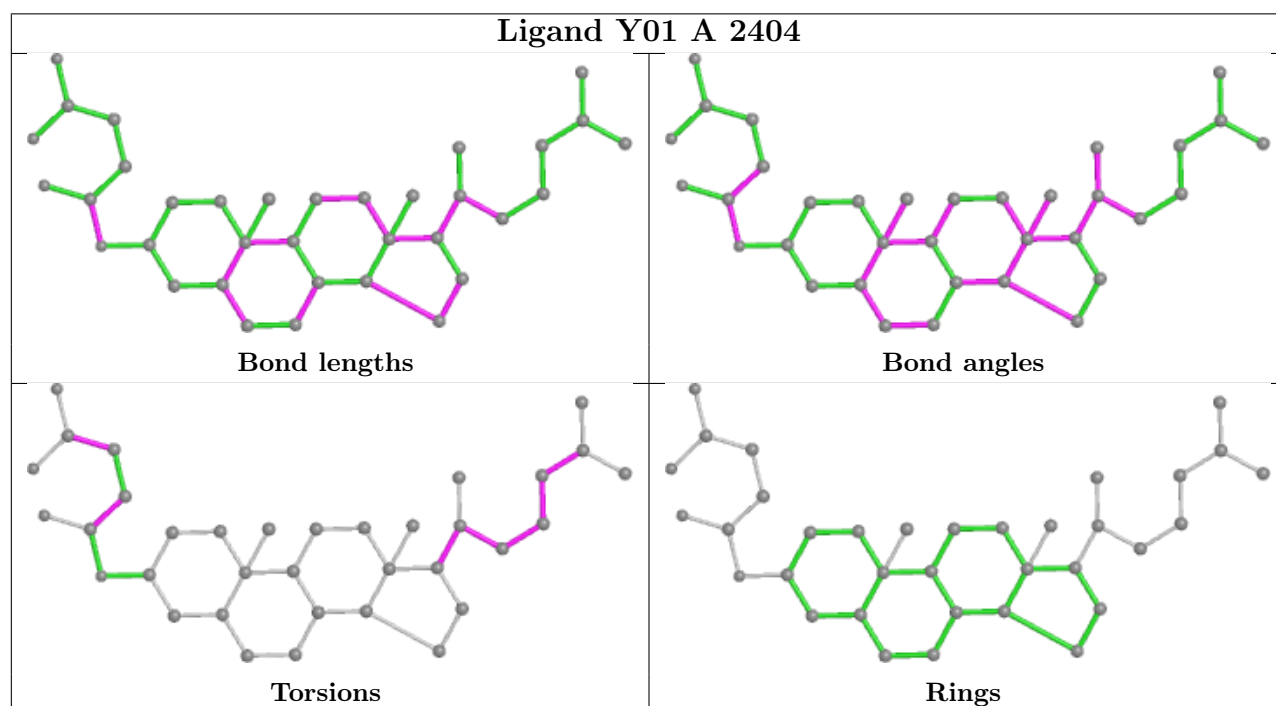
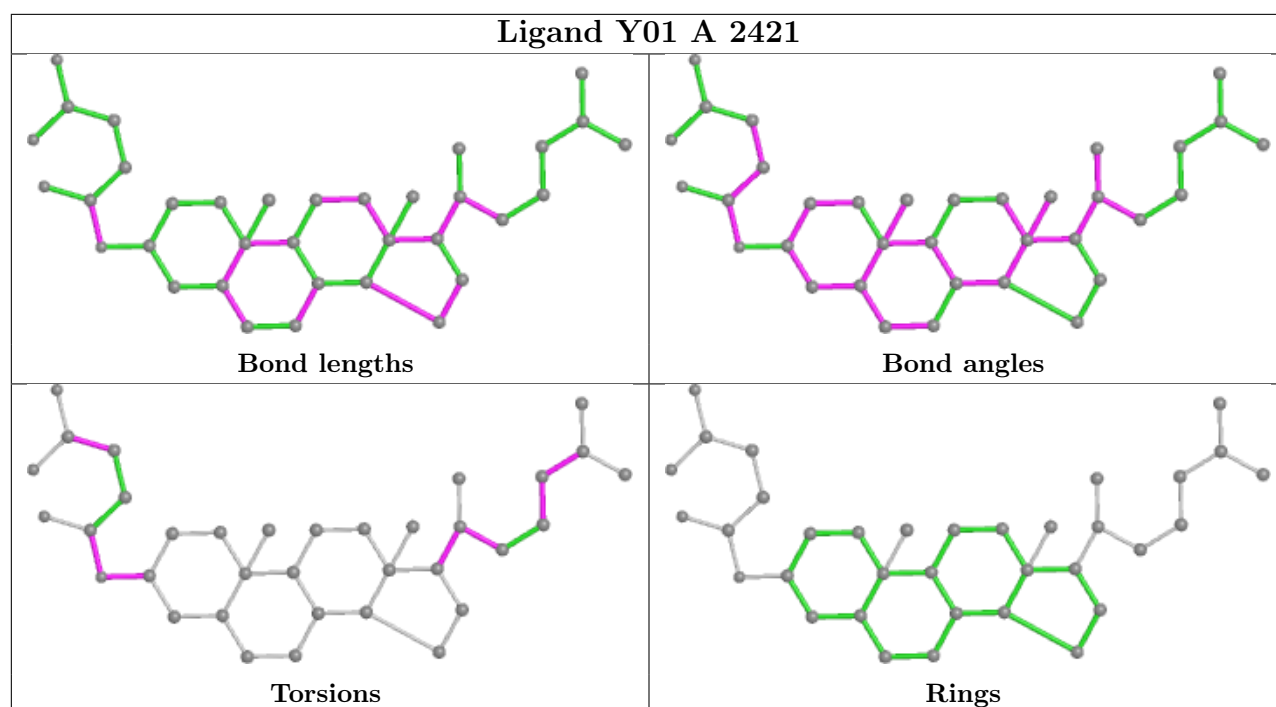
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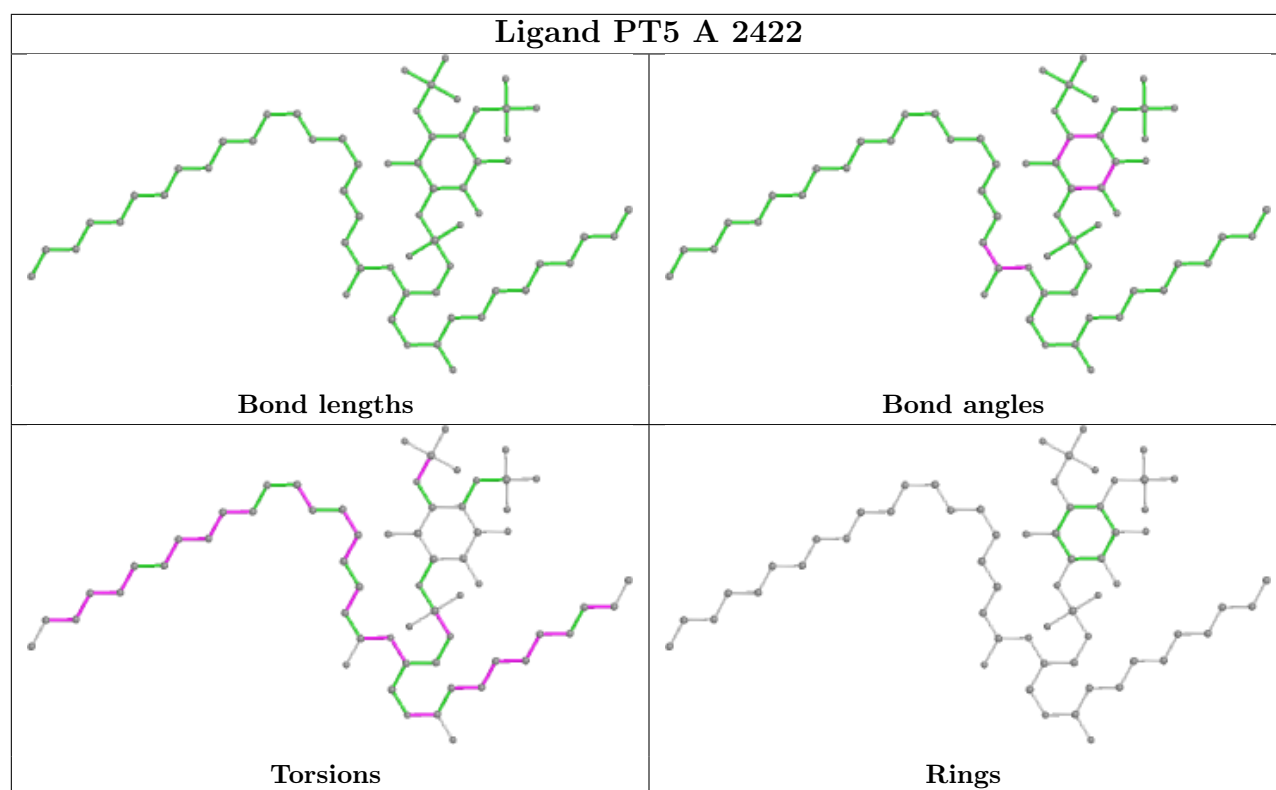
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2404	Y01	6	0
7	A	2420	R16	1	0
7	A	2405	R16	1	0
9	A	2422	PT5	4	0
7	A	2402	R16	1	0
7	A	2401	R16	2	0
11	B	1208	NAG	1	0

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







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.

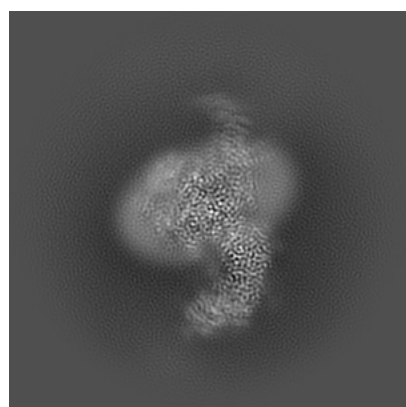
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31959. These allow visual inspection of the internal detail of the map and identification of artifacts.

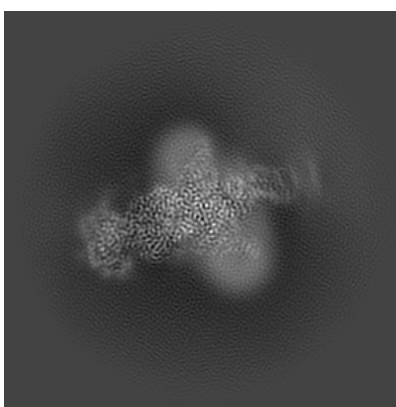
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

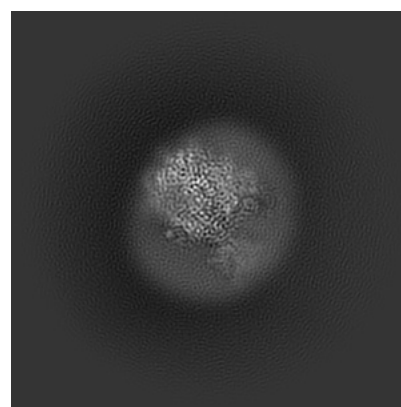
6.1.1 Primary map



X



Y

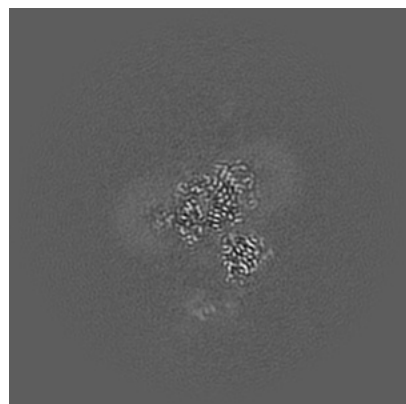


Z

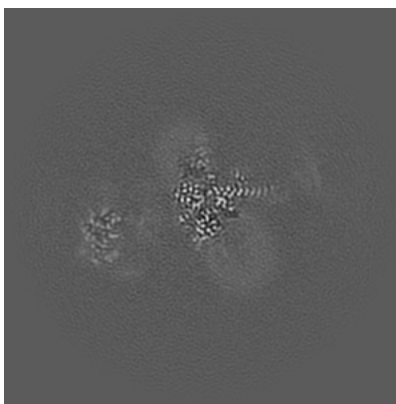
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

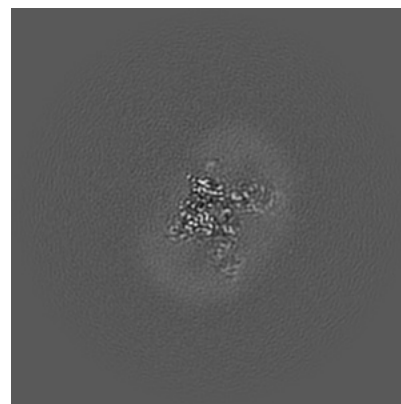
6.2.1 Primary map



X Index: 160



Y Index: 160

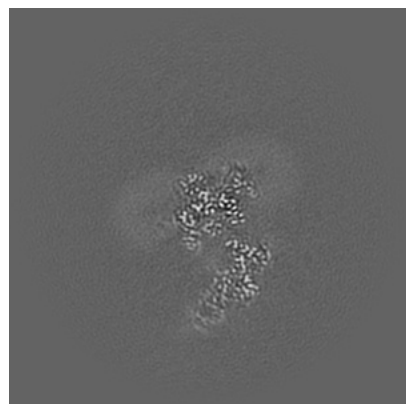


Z Index: 160

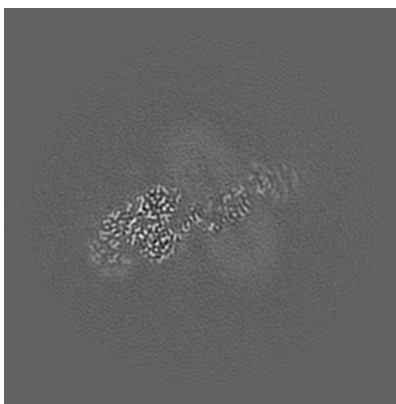
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

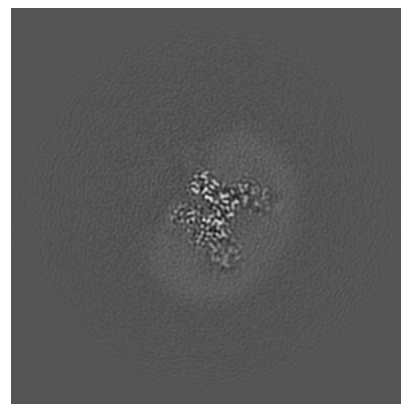
6.3.1 Primary map



X Index: 152



Y Index: 186

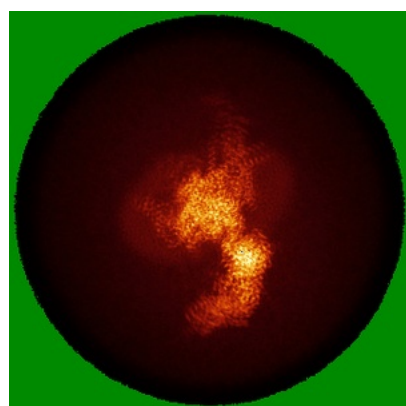


Z Index: 153

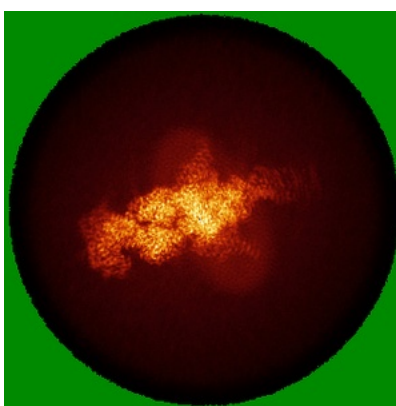
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

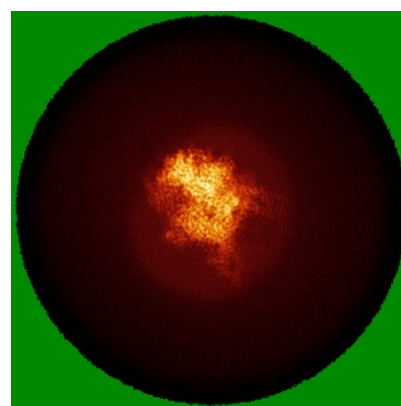
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

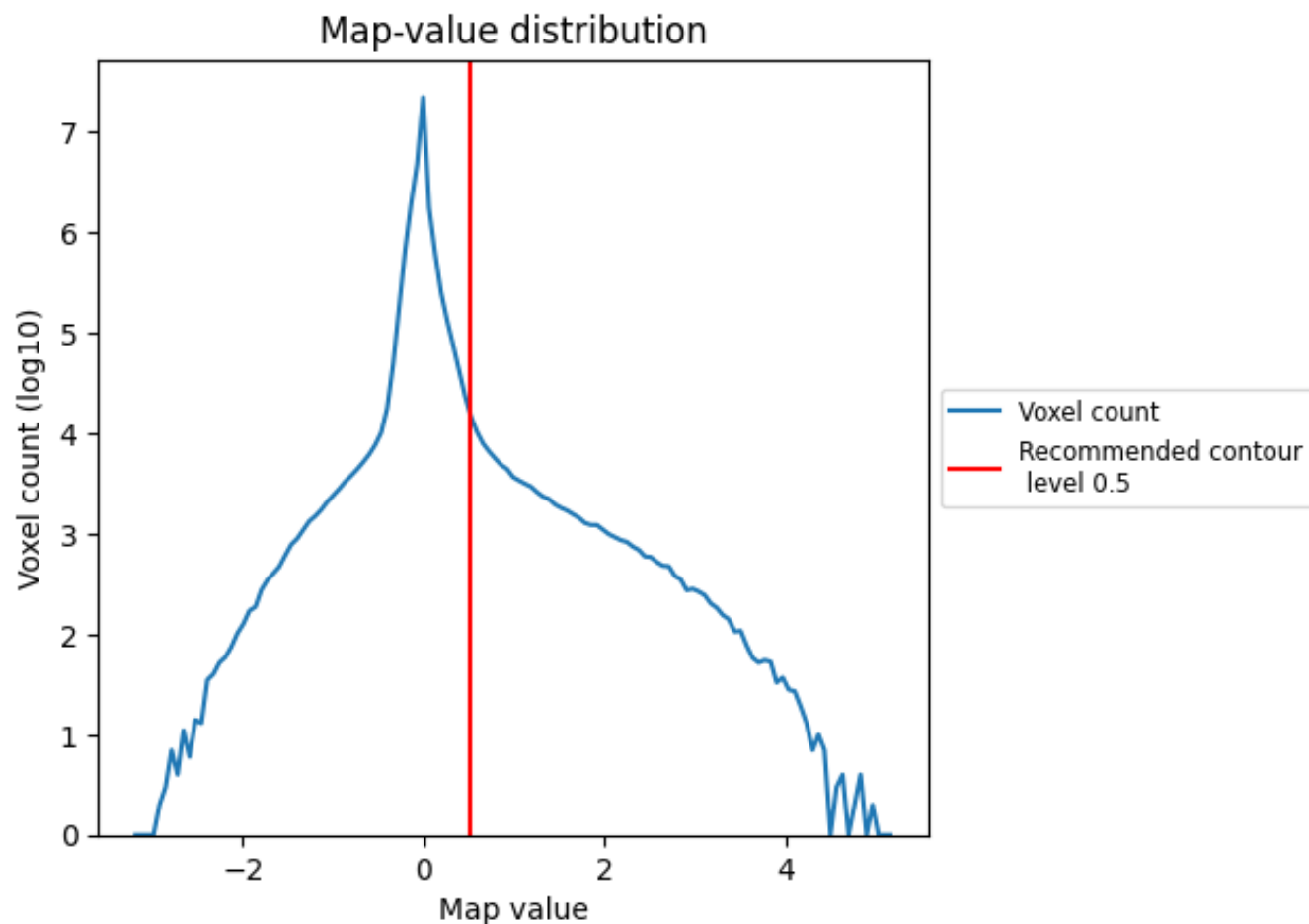
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

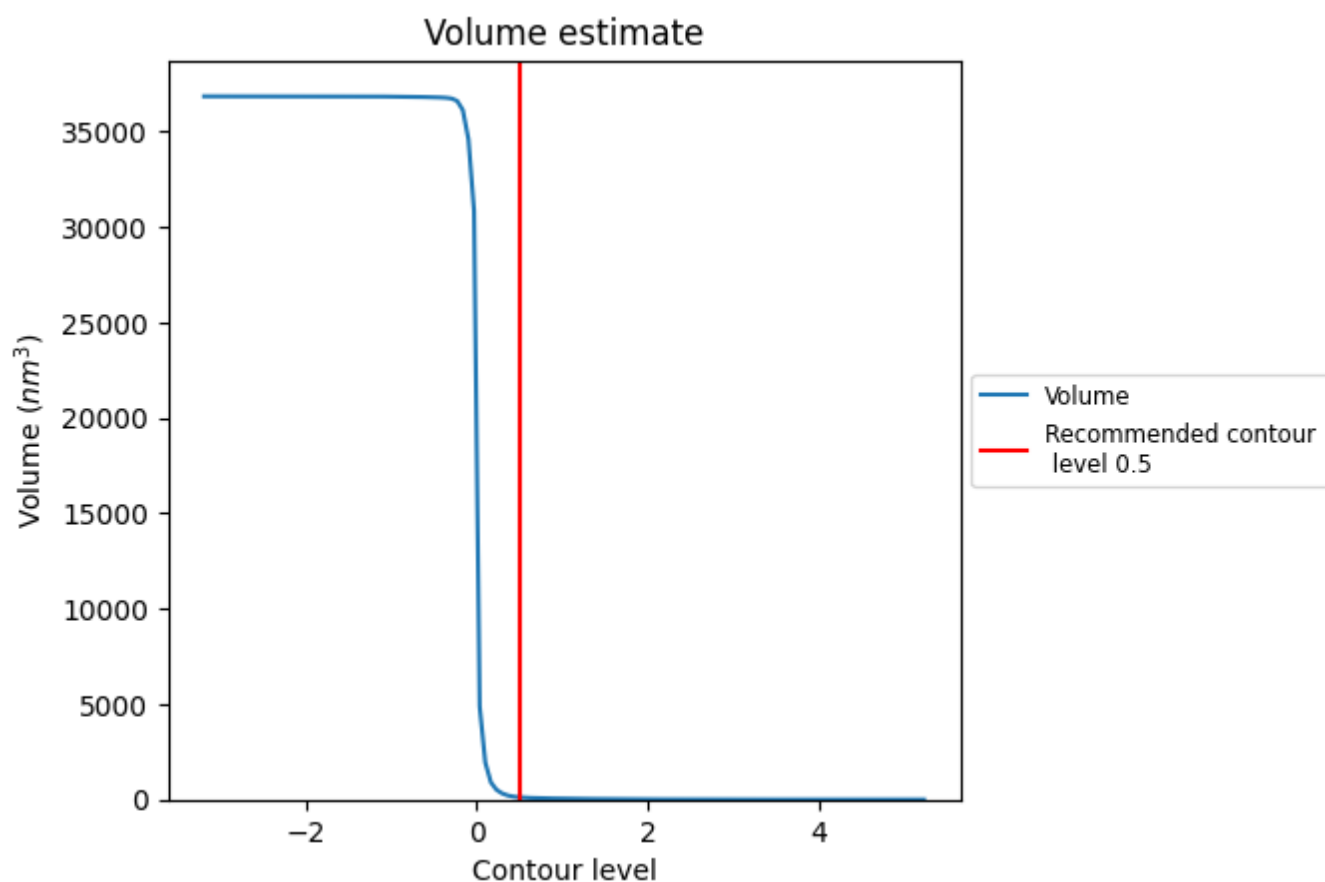
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

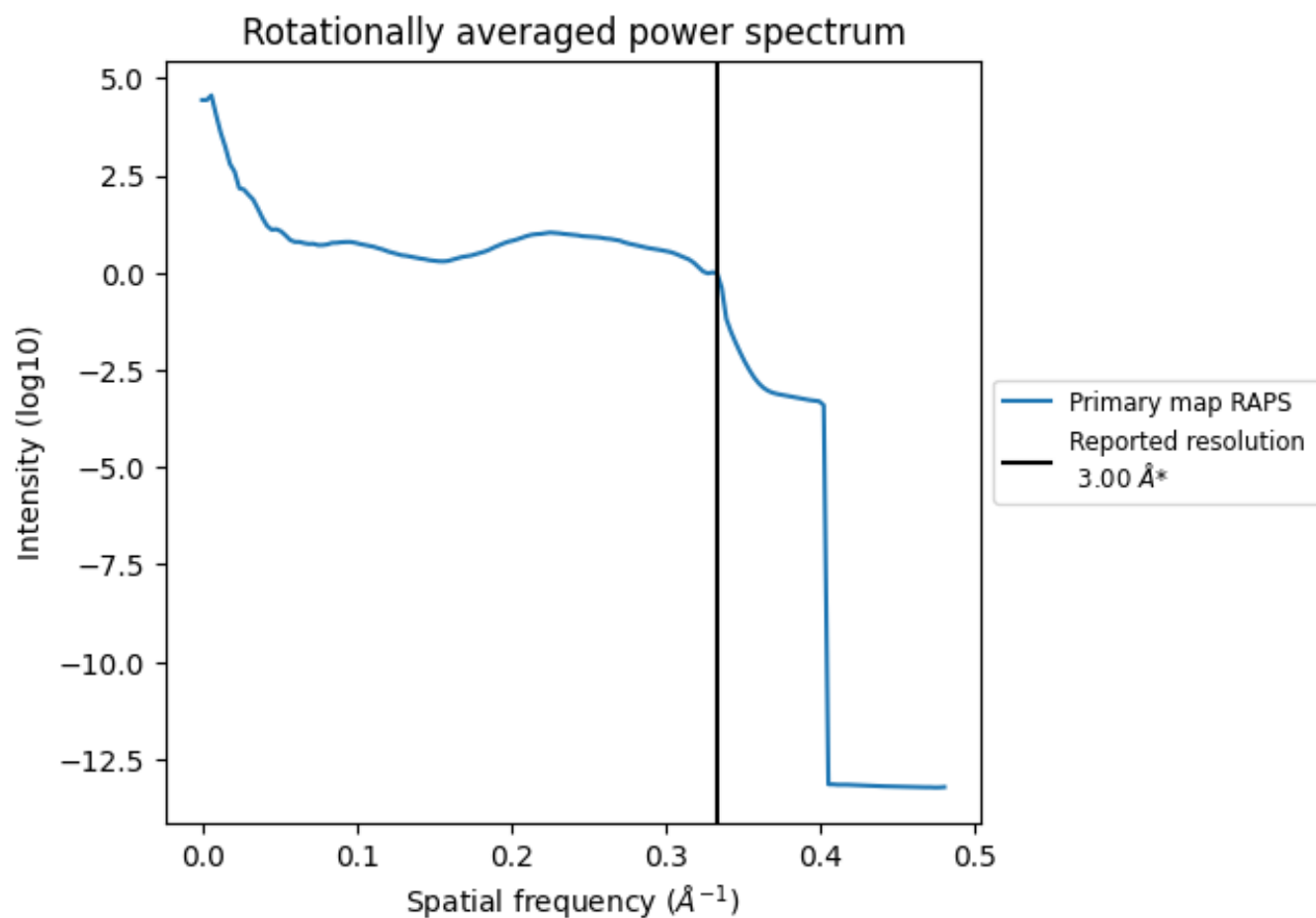
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

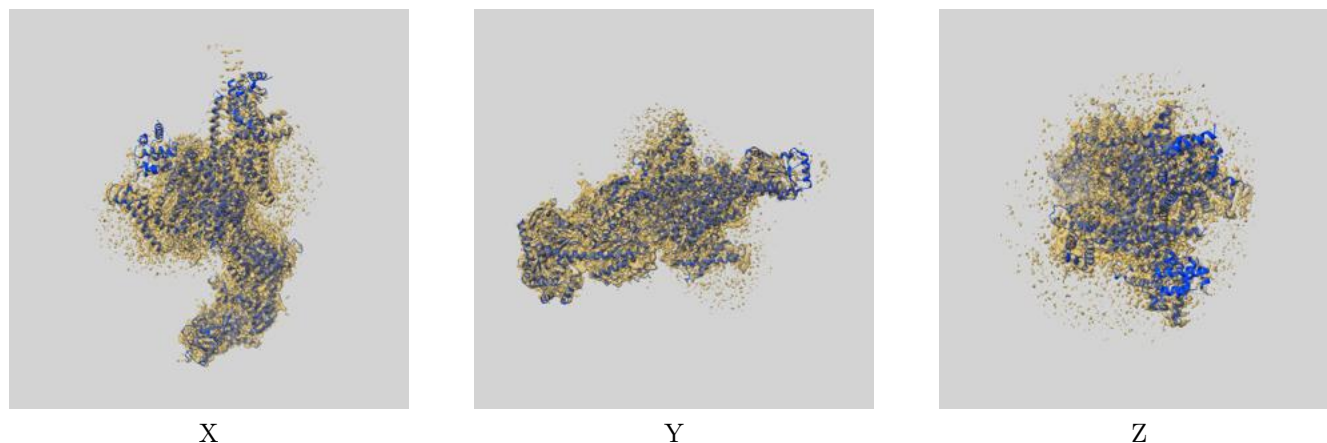
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

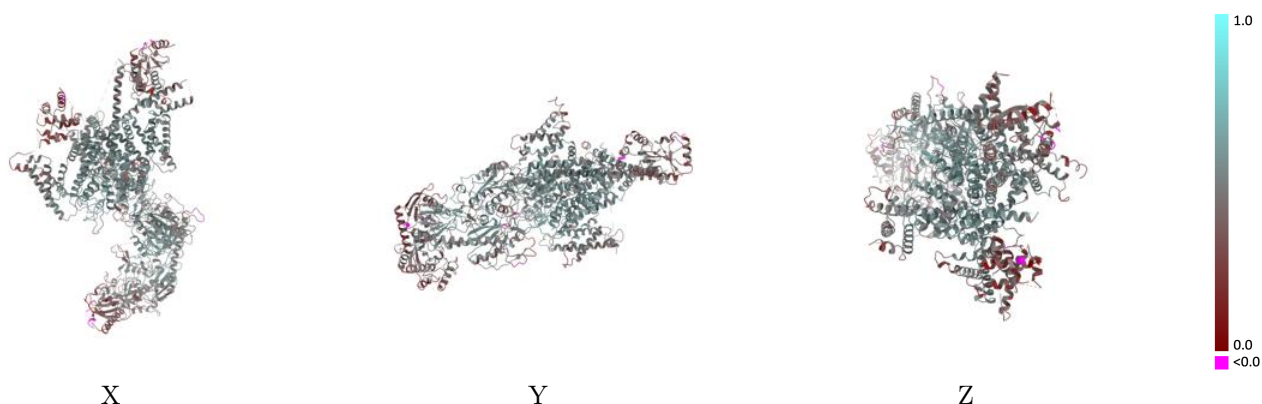
This section contains information regarding the fit between EMDB map EMD-31959 and PDB model 7VFU. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



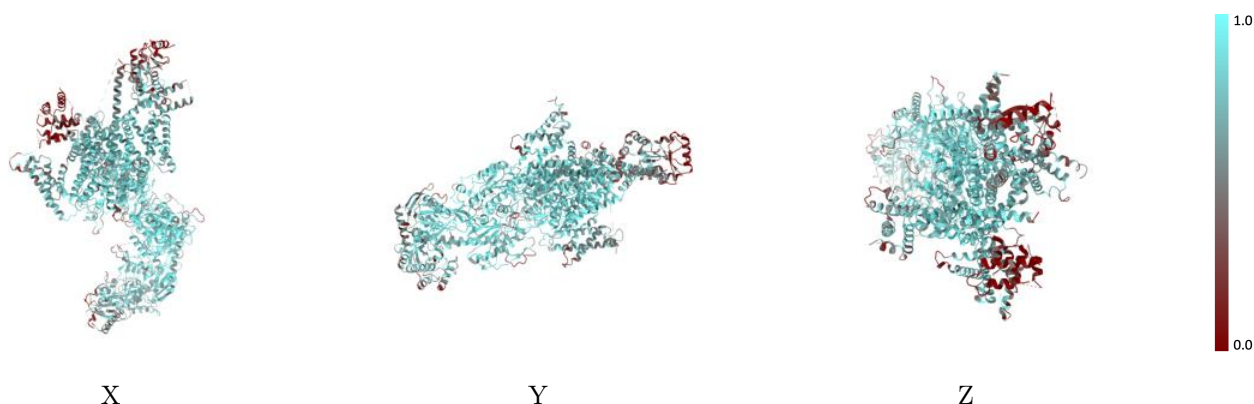
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



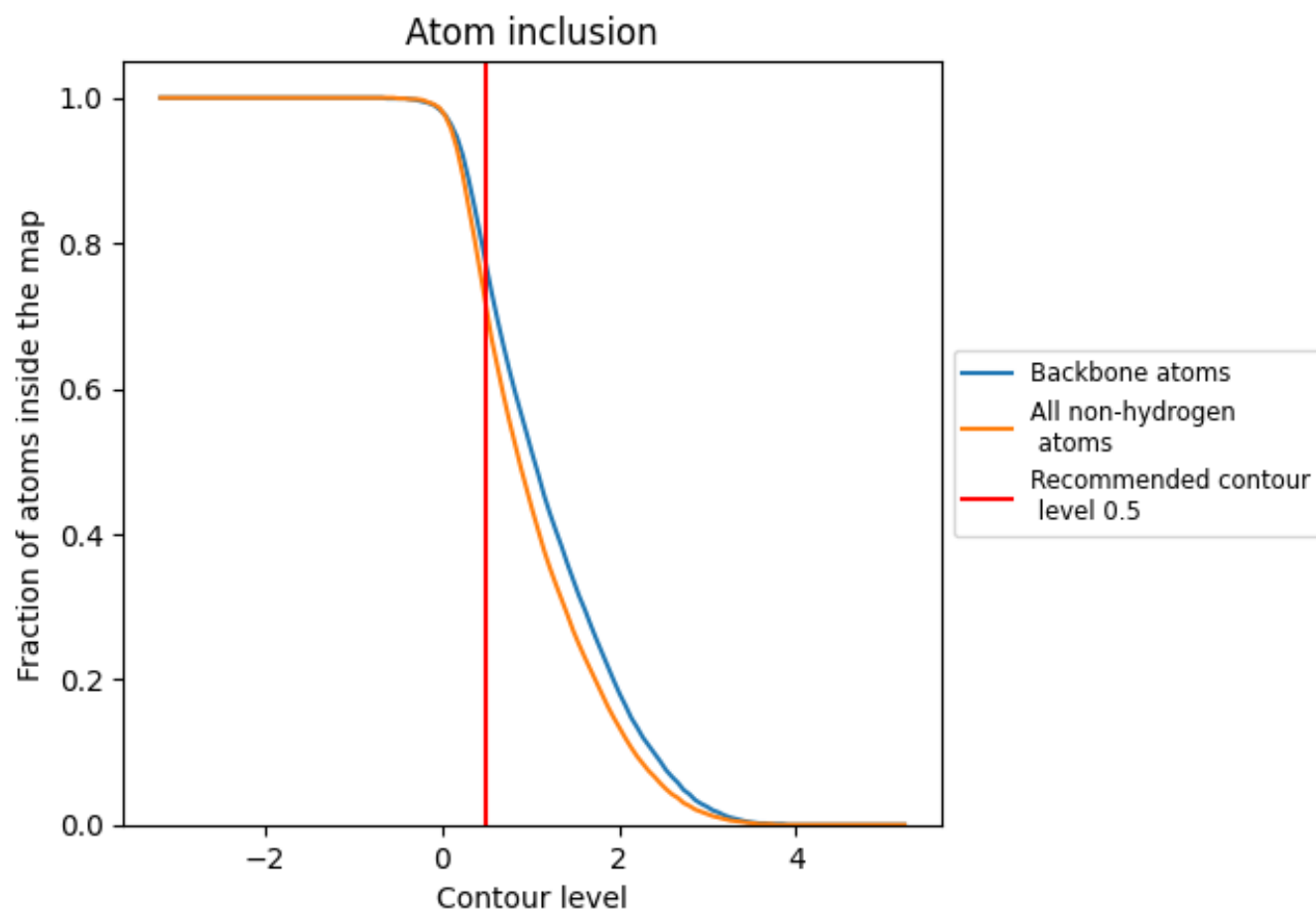
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 71% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7080	<div></div> 0.4740
A	<div></div> 0.7310	<div></div> 0.5100
B	<div></div> 0.7260	<div></div> 0.4390
C	<div></div> 0.4620	<div></div> 0.3630
D	<div></div> 0.4020	<div></div> 0.3790
E	<div></div> 0.8830	<div></div> 0.5680
F	<div></div> 0.7440	<div></div> 0.4340
G	<div></div> 0.4100	<div></div> 0.2720

1.0

0.0

<0.0