



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:46 PM UTC

PDB ID : 7VFW / pdb_00007vfw
EMDB ID : EMD-31961
Title : Human N-type voltage gated calcium channel CaV2.2-alpha2/delta1-beta1 complex, bound to CaV2.2-blocker1
Authors : Dong, Y.; Gao, Y.; Wang, Y.; Zhao, Y.
Deposited on : 2021-09-13
Resolution : 3.30 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:

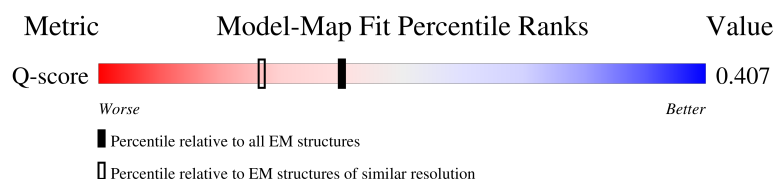
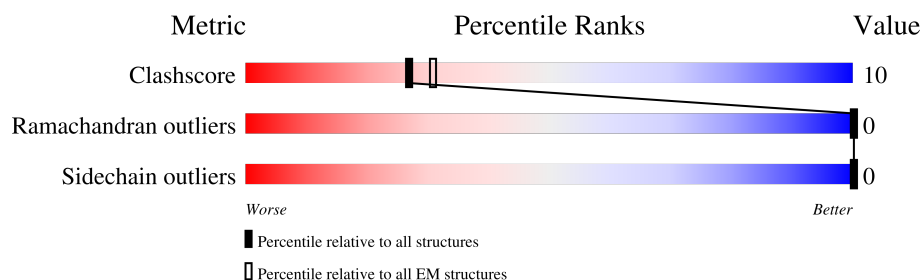
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	B	1103	
3	D	598	
4	C	3	

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Mol	Chain	Length	Quality of chain
4	E	3	 67%33%
5	F	3	 67%33%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 19746 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		

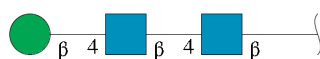
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	162	Total	C	N	O	S	0	0
			1259	805	217	232	5		

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



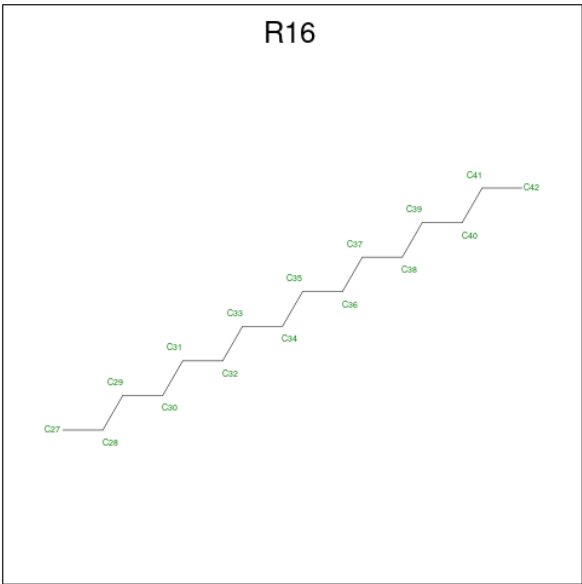
Mol	Chain	Residues	Atoms				AltConf	Trace
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

- Molecule 6 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			16	16	
6	A	1	Total	C	0
			16	16	
6	A	1	Total	C	0
			16	16	
6	A	1	Total	C	0
			16	16	
6	A	1	Total	C	0
			16	16	
6	A	1	Total	C	0
			11	11	
6	A	1	Total	C	0
			13	13	

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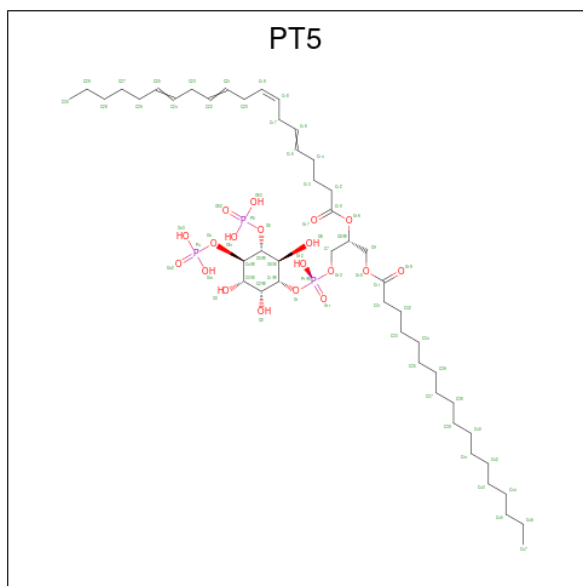
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C 15 15	0
6	A	1	Total C 13 13	0
6	A	1	Total C 12 12	0
6	A	1	Total C 15 15	0
6	A	1	Total C 13 13	0
6	A	1	Total C 16 16	0
6	A	1	Total C 16 16	0

- # Y01

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

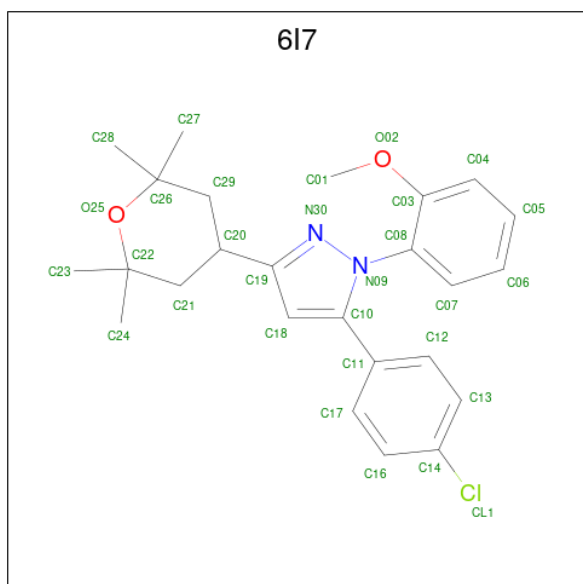
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PDB
PROTEIN DATA BANK

aenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	O	P	0
			62	40	19	3	

- Molecule 9 is 5-(4-chlorophenyl)-1-(2-methoxyphenyl)-3-(2,2,6,6-tetramethyloxan-4-yl)pyrazole (CCD ID: 6I7) (formula: $C_{25}H_{29}ClN_2O_2$) (labeled as "Ligand of Interest" by depositor).

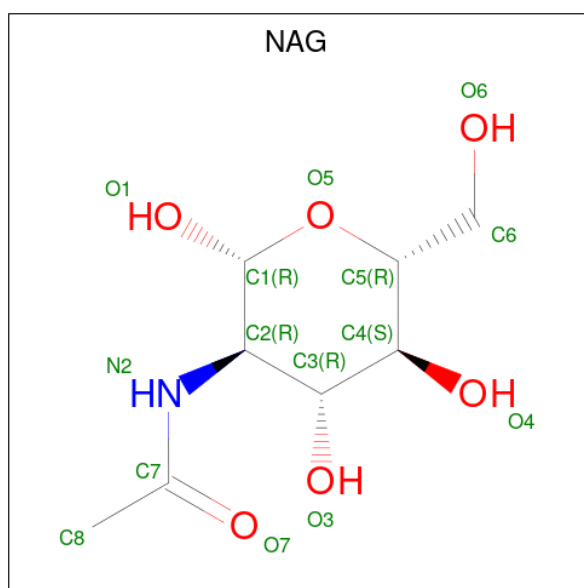


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Cl	N	O	0
			30	25	1	2	2	

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Ca	0
			1	1	
10	B	1	Total	Ca	0
			1	1	

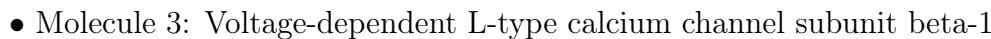
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	
11	B	1	Total	C	N	O	0
			14	8	1	5	

ARG	ARG	LEU	ARG	GLN	THR	GLY	LEU	SER	I1612	T1485	M1369	L1222	ASP	GLN
VAL	VAL	ALA	VAL	LEU	THR	GLY	PHE	LEU	Y1613	V1486	ASP	D1223	VAL	PRO
ASN	ASN	GLY	ALA	HIS	GLN	ASP	F1750	GLY	D1628	V1487	MET	I1225	ASP	GLU
GLY	GLY	THR	THR	PRO	LEU	THR	M1752	PRO	R1634	K1491	SER	S1228	ARG	ALA
THR	THR	ASP	LYS	LYS	LYS	LYS	H1755	GLY	M1646	F1492	GLY	V1232	ASN	ASN
LEU	LEU	ALA	ALA	ALA	ALA	ALA	M1756	LEU	R1650	D1494	PRO	I1247	GLN	GLN
PRO	PRO	ASP	THR	THR	THR	THR	S1757	GLY	R1654	A1495	ARG	K1248	ARG	ARG
GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLY	G1654	P1496	ILE	S1239	ASN	ASN
THR	THR	THR	THR	THR	THR	THR	PRO	GLY	G1654	Y1497	VAL	G1240	THR	THR
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLY	LEU	I1660	E1498	PRO	G1241	ARG	ARG
PRO	PRO	PRO	PRO	PRO	PRO	PRO	LEU	LEU	E1499	F1401	TYR	K1242	MET	MET
ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	LEU	F1510	V1402	SER	I1247	GLY	GLY
VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	E1672	F1403	THR	K1248	SER	SER
GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	LYS	M1675	P1404	THR	I1251	GLN	GLN
ARG	ARG	ARG	ARG	ARG	ARG	ARG	CYS	CYS	A1676	F1405	PHE	T1261	PRO	PRO
SER	SER	SER	SER	SER	SER	SER	PRO	PRO	S1681	F1406	CYS	I1262	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	ALA	E1517	M1409	LEU	V1255	LEU	LEU
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ARG	ARG	C1518	A1413	PRO	P1258	PRO	PRO
GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	VAL	V1519	L1414	THR	L1259	ASN	ASN
THR	THR	THR	THR	THR	THR	THR	ALA	ALA	I1520	L1414	THR	K1260	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	ALA	ALA	K1521	L1414	THR	T1261	LEU	LEU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	LYS	I1522	L1414	THR	I1262	PRO	PRO
VAL	VAL	VAL	VAL	VAL	VAL	VAL	ARG	ARG	I1523	L1414	THR	I1262	ILE	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	LEU	LEU	F1538	L1414	THR	K1269	MET	MET
GLN	GLN	GLN	GLN	GLN	GLN	GLN	VAL	VAL	T1542	L1414	THR	F1272	LEU	LEU
THR	THR	THR	THR	THR	THR	THR	ALA	ALA	S1546	L1414	THR	F1272	THR	THR
SER	SER	SER	SER	SER	SER	SER	ALA	ALA	T1558	L1414	THR	N1284	GLY	GLY
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	I1562	L1414	THR	I1285	LEU	LEU
ILE	ILE	ILE	ILE	ILE	ILE	ILE	LEU	LEU	S1565	L1414	THR	Y1289	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ASP	R1568	L1414	THR	A1297	ALA	ALA
ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	R1574	L1414	THR	V1301	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	R1574	L1414	THR	V1301	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR	THR	Q1581	L1414	THR	F1304	PRO	PRO
GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR	THR	G1582	L1414	THR	K1305	SER	SER
LYS	LYS	LYS	LYS	LYS	LYS	LYS	THR	THR	Y1583	L1414	THR	D1313	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	T1584	L1414	THR	E1332	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	I1585	L1414	THR	Y1188	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	THR	R1586	L1414	THR	V1193	ASP	ASP
SER	SER	SER	SER	SER	SER	SER	THR	THR	I1587	L1414	THR	R1339	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	L1588	L1414	THR	N1350	SER	SER
THR	THR	THR	THR	THR	THR	THR	THR	THR	L1589	L1414	THR	F1359	GLY	GLY
GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	W1590	L1414	THR	T1363	LYS	LYS
LEU	LEU	LEU	LEU	LEU	LEU	LEU	THR	THR	T1591	L1414	THR	K1201	GLY	GLY
SER	SER	SER	SER	SER	SER	SER	THR	THR	S1595	L1414	THR	M1202	VAL	VAL
ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	THR	M1608	L1414	THR	E1365	GLY	GLY
PRO	PRO	PRO	PRO	PRO	PRO	PRO	THR	THR	L1609	L1414	THR	W1367	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	THR	T1609	L1414	THR	P1368	ALA	ALA

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399567	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	4.835	Depositor
Minimum map value	-2.541	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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: R16, 6I7, BMA, PT5, CA, Y01, NAG

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	0.20	0/10448	0.45	2/14152 (0.0%)
2	B	0.21	0/7799	0.44	1/10578 (0.0%)
3	D	0.16	0/1280	0.43	0/1729
All	All	0.20	0/19527	0.44	3/26459 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	CYS	CA-C-N	15.17	145.29	121.03
1	A	253	CYS	C-N-CA	15.17	145.29	121.03
2	B	1069	THR	CB-CA-C	-5.76	104.14	111.22

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	190	0
2	B	7637	0	7426	153	0
3	D	1259	0	1254	46	0
4	C	39	0	34	0	0
4	E	39	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	39	0	34	0	0
6	A	220	0	440	12	0
7	A	105	0	147	6	0
8	A	62	0	63	7	0
9	A	30	0	0	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	112	0	104	3	0
All	All	19746	0	19715	389	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 (389) 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:679:VAL:CG2	1:A:683:MET:HE1	1.73	1.17
1:A:679:VAL:HG23	1:A:683:MET:HE1	1.02	0.99
2:B:100:LEU:HB3	2:B:488:MET:HE2	1.54	0.90
1:A:679:VAL:HG23	1:A:683:MET:CE	1.97	0.85
1:A:1800:ARG:HD2	1:A:1821:LEU:HD11	1.58	0.85
1:A:1350:ASN:HD21	7:A:2403:Y01:HAR2	1.42	0.84
3:D:243:GLU:H	3:D:363:GLN:HE22	1.26	0.82
2:B:85:ASP:HB3	2:B:500:LEU:HD22	1.65	0.79
2:B:994:LEU:HB3	2:B:1001:ARG:HB2	1.66	0.77
1:A:679:VAL:CG2	1:A:683:MET:CE	2.61	0.76
2:B:149:PHE:HB3	2:B:158:GLN:HB3	1.65	0.76
1:A:595:LEU:HB3	8:A:2419:PT5:H24	1.68	0.76
1:A:1706:VAL:O	1:A:1710:ASN:ND2	2.19	0.75
1:A:381:ILE:HD13	3:D:350:LYS:HD2	1.69	0.75
2:B:104:ALA:HB2	2:B:189:LEU:HD21	1.71	0.72
1:A:363:ARG:NH2	1:A:717:GLU:OE2	2.24	0.71
2:B:508:PRO:HG2	2:B:764:TYR:HE2	1.56	0.70
1:A:229:LEU:HG	1:A:347:MET:HE1	1.72	0.70
3:D:328:HIS:HB3	3:D:331:GLN:HB2	1.73	0.70
1:A:1478:MET:HE3	1:A:1581:GLN:HG3	1.74	0.69
1:A:363:ARG:NH1	1:A:714:ASN:OD1	2.25	0.69
1:A:1400:PHE:HA	1:A:1404:PRO:HD2	1.74	0.69
1:A:1650:ARG:HH11	1:A:1660:ILE:HD11	1.58	0.68
3:D:244:VAL:HG21	3:D:356:ILE:HD13	1.76	0.68
3:D:353:GLN:HE22	3:D:357:LYS:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:PRO:HG2	2:B:764:TYR:CE2	2.29	0.67
2:B:751:ASN:O	2:B:753:GLN:NE2	2.30	0.65
1:A:1700:LEU:HD13	9:A:2420:6I7:C27	2.27	0.65
2:B:644:TYR:O	2:B:647:THR:OG1	2.13	0.65
3:D:389:LEU:HD12	3:D:397:ALA:HB1	1.79	0.65
1:A:229:LEU:HB2	1:A:1585:ILE:HD11	1.78	0.65
2:B:57:LEU:HD23	2:B:798:VAL:HG11	1.78	0.65
1:A:1517:GLU:OE2	1:A:1521:LYS:NZ	2.20	0.64
2:B:90:LEU:HD12	2:B:615:THR:HG21	1.80	0.64
1:A:187:ASP:HA	1:A:191:LEU:HD23	1.79	0.64
2:B:423:THR:HG23	2:B:426:TYR:HE2	1.63	0.64
1:A:376:ARG:NH2	1:A:721:ASP:OD2	2.31	0.64
1:A:311:ILE:HD12	1:A:343:GLY:HA3	1.79	0.64
1:A:1262:ILE:HD11	1:A:1272:PHE:HB2	1.80	0.63
3:D:229:MET:HE3	3:D:318:LEU:HA	1.80	0.63
1:A:1403:PHE:HB2	1:A:1404:PRO:HD3	1.79	0.63
2:B:646:GLU:HA	2:B:649:LYS:NZ	2.13	0.63
2:B:224:VAL:HG23	2:B:225:ASP:H	1.63	0.63
1:A:1688:PHE:O	1:A:1692:ILE:HG12	1.99	0.63
1:A:1285:ILE:HG13	1:A:1414:LEU:HD11	1.81	0.63
2:B:237:ASP:OD2	2:B:424:GLN:NE2	2.32	0.63
2:B:368:ARG:HG2	2:B:398:PRO:HB3	1.80	0.63
2:B:204:LEU:HD13	2:B:456:LEU:HD13	1.81	0.62
1:A:1681:SER:HB2	6:A:2401:R16:H412	1.81	0.62
1:A:1304:PHE:HE1	1:A:1392:LEU:HD13	1.65	0.62
1:A:1613:TYR:O	1:A:1687:TYR:OH	2.16	0.61
1:A:85:ARG:HB3	1:A:89:LYS:HZ3	1.65	0.61
2:B:36:TRP:HH2	2:B:829:SER:HA	1.66	0.61
1:A:119:PRO:HD2	2:B:263:SER:HA	1.82	0.61
1:A:1486:VAL:HG13	7:A:2409:Y01:HAC3	1.83	0.60
2:B:721:SER:O	2:B:724:LYS:HE3	2.01	0.60
2:B:105:GLU:OE2	2:B:442:LYS:NZ	2.33	0.60
1:A:285:GLU:OE2	1:A:1493:TYR:OH	2.18	0.60
1:A:715:ALA:O	1:A:719:THR:HG23	2.02	0.60
2:B:357:ILE:HG21	2:B:359:MET:HE2	1.83	0.60
2:B:775:PHE:CD1	2:B:794:VAL:HG22	2.37	0.59
1:A:250:HIS:NE2	1:A:298:ASP:OD2	2.27	0.59
2:B:885:HIS:O	2:B:889:ILE:HD12	2.03	0.59
2:B:1015:PHE:HE2	2:B:1017:MET:HE2	1.67	0.59
1:A:108:ASN:ND2	1:A:198:ARG:HD3	2.18	0.59
1:A:596:ARG:HH21	8:A:2419:PT5:H2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:MET:O	1:A:1612:ILE:HG12	2.03	0.58
3:D:237:PRO:HG2	3:D:245:THR:HG23	1.85	0.58
1:A:1313:ASP:OD2	1:A:1339:ARG:NH2	2.35	0.58
1:A:135:PRO:HA	1:A:138:ILE:HG22	1.86	0.58
1:A:1752:MET:O	1:A:1756:MET:N	2.36	0.58
1:A:229:LEU:HD21	1:A:1589:LEU:HD21	1.86	0.58
1:A:546:PHE:HB2	8:A:2419:PT5:H17	1.85	0.58
1:A:302:PHE:O	1:A:306:THR:HG23	2.04	0.58
1:A:485:TYR:OH	1:A:584:ARG:O	2.21	0.57
2:B:997:GLY:N	2:B:1026:CYS:SG	2.75	0.57
1:A:1365:GLU:CD	1:A:1654:GLY:O	2.48	0.57
2:B:726:ILE:HB	2:B:729:VAL:HG22	1.87	0.57
1:A:102:LEU:O	1:A:106:ILE:HD12	2.05	0.57
2:B:128:LYS:NZ	2:B:234:ASP:OD2	2.36	0.56
2:B:57:LEU:HD13	2:B:715:LEU:HD22	1.87	0.56
2:B:713:ASN:HA	2:B:716:VAL:HG12	1.87	0.56
1:A:85:ARG:HB3	1:A:89:LYS:NZ	2.19	0.56
1:A:1161:ALA:O	1:A:1165:ILE:HG12	2.06	0.56
2:B:226:ASN:HB3	2:B:234:ASP:HB2	1.88	0.56
2:B:442:LYS:NZ	2:B:465:PRO:O	2.37	0.56
1:A:176:THR:HG21	1:A:194:VAL:HG11	1.86	0.56
1:A:1477:ILE:O	1:A:1481:ILE:HG12	2.06	0.56
1:A:529:MET:SD	1:A:554:ILE:HD11	2.47	0.55
1:A:1159:VAL:HG21	1:A:1193:VAL:HG11	1.87	0.55
1:A:1198:MET:O	1:A:1202:MET:HG2	2.06	0.55
1:A:213:LEU:HD13	1:A:615:LEU:HD13	1.88	0.55
2:B:646:GLU:HA	2:B:649:LYS:HZ3	1.70	0.55
2:B:896:LYS:HB3	2:B:977:GLU:OE2	2.06	0.55
2:B:994:LEU:N	2:B:1001:ARG:O	2.30	0.55
2:B:1042:ASN:ND2	2:B:1045:ASP:OD2	2.39	0.55
3:D:346:ILE:HD11	3:D:352:LEU:HD12	1.88	0.55
3:D:240:LYS:NZ	3:D:326:ILE:O	2.27	0.55
2:B:819:ASN:HA	2:B:822:ILE:HG22	1.89	0.54
1:A:285:GLU:HG3	1:A:286:TYR:H	1.72	0.54
1:A:122:ASP:HB2	2:B:262:GLY:HA3	1.90	0.54
1:A:1546:SER:OG	1:A:1574:ARG:NH1	2.39	0.54
2:B:537:PRO:HB3	2:B:972:GLN:HB2	1.89	0.54
1:A:246:MET:HE1	1:A:1491:LYS:HE2	1.89	0.54
1:A:1223:ASP:OD1	1:A:1260:LYS:NZ	2.33	0.54
1:A:1228:SER:O	1:A:1232:VAL:HG23	2.07	0.54
1:A:1388:TYR:CD2	1:A:1389:ARG:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:HG22	1:A:567:LYS:HG3	1.90	0.54
2:B:884:ARG:HG3	2:B:1031:LEU:HD11	1.89	0.54
3:D:344:ILE:HA	3:D:389:LEU:HB2	1.89	0.54
1:A:299:ASN:HB3	1:A:302:PHE:HD2	1.73	0.53
2:B:296:SER:HA	2:B:332:ASP:HB2	1.90	0.53
2:B:604:ASN:OD1	11:B:1205:NAG:N2	2.41	0.53
3:D:268:ARG:HA	3:D:322:ASP:HB3	1.91	0.53
3:D:255:PHE:HA	3:D:258:HIS:CE1	2.43	0.53
1:A:1824:GLU:O	1:A:1828:VAL:HG22	2.09	0.53
2:B:772:ASN:HD21	2:B:1011:THR:N	2.05	0.53
2:B:128:LYS:HB3	2:B:227:SER:HA	1.91	0.53
3:D:391:GLU:HB2	3:D:397:ALA:HB2	1.90	0.53
1:A:1248:LYS:O	1:A:1252:VAL:HG23	2.08	0.53
2:B:193:PHE:HB3	2:B:218:TYR:HB2	1.91	0.53
2:B:658:TYR:HD2	2:B:749:GLY:HA3	1.73	0.52
2:B:494:LEU:HD11	2:B:522:LEU:O	2.09	0.52
2:B:663:PRO:HD3	2:B:756:PRO:HB2	1.89	0.52
1:A:130:LEU:O	1:A:133:THR:HG22	2.09	0.52
2:B:285:ASP:O	2:B:309:GLN:NE2	2.37	0.52
3:D:253:PHE:HE1	3:D:320:ALA:HB1	1.74	0.52
1:A:616:LEU:HD11	1:A:703:VAL:HG21	1.92	0.52
2:B:58:VAL:HG13	2:B:800:ILE:HG22	1.92	0.52
2:B:179:VAL:HG13	2:B:214:LEU:HD21	1.92	0.52
1:A:1650:ARG:NH1	1:A:1660:ILE:HD11	2.25	0.52
2:B:363:ASP:OD1	2:B:364:GLY:N	2.41	0.52
1:A:301:LEU:HB3	6:A:2407:R16:H322	1.92	0.52
2:B:160:SER:HB3	2:B:220:ALA:HB3	1.91	0.52
1:A:400:LEU:HD21	1:A:469:LYS:HB3	1.92	0.51
2:B:38:ASP:O	2:B:41:GLN:HG3	2.09	0.51
1:A:184:THR:OG1	1:A:187:ASP:OD2	2.28	0.51
2:B:511:TYR:OH	2:B:565:GLU:OE2	2.19	0.51
2:B:204:LEU:HD11	2:B:493:SER:HB2	1.92	0.51
2:B:407:LYS:HD2	2:B:1068:TYR:CE1	2.46	0.51
2:B:84:ARG:HG3	11:B:1206:NAG:H81	1.91	0.51
2:B:702:ILE:HA	2:B:705:VAL:HG12	1.92	0.51
2:B:74:ASN:ND2	2:B:77:GLN:OE1	2.43	0.51
2:B:562:LEU:HD12	2:B:1051:ARG:HE	1.76	0.51
2:B:59:ASP:O	2:B:63:LYS:HB2	2.10	0.51
1:A:1196:PHE:O	1:A:1200:ILE:HG12	2.11	0.50
2:B:667:CYS:HB2	2:B:670:LEU:HD13	1.93	0.50
2:B:514:ALA:HB3	2:B:522:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLU:HG2	2:B:192:VAL:HG21	1.92	0.50
2:B:185:TRP:HA	11:B:1209:NAG:H82	1.92	0.50
2:B:773:TYR:CE1	2:B:796:LYS:HD2	2.46	0.50
1:A:700:LEU:HD21	1:A:1405:PHE:CZ	2.47	0.50
1:A:285:GLU:HG3	1:A:286:TYR:N	2.26	0.50
1:A:1711:PHE:O	1:A:1715:THR:OG1	2.28	0.50
3:D:253:PHE:HZ	3:D:266:ILE:HG23	1.77	0.50
2:B:601:ASP:OD1	2:B:602:LYS:N	2.44	0.50
1:A:330:THR:HG1	1:A:331:TRP:CD1	2.30	0.50
2:B:63:LYS:HD2	2:B:64:TYR:CZ	2.47	0.50
2:B:167:HIS:CE1	2:B:236:TYR:HD2	2.30	0.50
3:D:352:LEU:O	3:D:356:ILE:HG12	2.11	0.50
2:B:647:THR:HG21	2:B:713:ASN:HD22	1.75	0.49
3:D:391:GLU:HG2	3:D:396:ASP:HB3	1.94	0.49
2:B:592:VAL:HG11	2:B:605:ARG:HH21	1.77	0.49
1:A:1304:PHE:CE1	1:A:1392:LEU:HD13	2.47	0.49
1:A:1675:ASN:OD1	1:A:1676:ALA:N	2.46	0.49
1:A:1752:MET:HE3	1:A:1756:MET:HA	1.93	0.49
2:B:36:TRP:O	2:B:39:LYS:HG2	2.13	0.49
2:B:631:ILE:O	2:B:704:ARG:NH1	2.46	0.49
1:A:302:PHE:CE1	1:A:683:MET:HE3	2.47	0.49
1:A:317:THR:HG21	1:A:1650:ARG:HG3	1.93	0.49
1:A:660:LEU:O	1:A:697:ASN:ND2	2.44	0.49
3:D:253:PHE:CZ	3:D:266:ILE:HG23	2.48	0.49
2:B:1015:PHE:CE2	2:B:1017:MET:HE2	2.46	0.48
3:D:387:ILE:HD11	3:D:404:TYR:CD1	2.48	0.48
2:B:709:ALA:O	2:B:742:ARG:NH1	2.45	0.48
1:A:1495:ALA:HB1	1:A:1499:TYR:HB3	1.95	0.48
1:A:1728:GLU:O	1:A:1732:VAL:HG23	2.13	0.48
2:B:66:ASP:OD1	2:B:66:ASP:N	2.45	0.48
1:A:1240:LYS:HG3	1:A:1242:LYS:H	1.79	0.48
2:B:768:LEU:O	2:B:808:LYS:NZ	2.39	0.48
1:A:1185:TYR:HA	1:A:1188:TYR:HD2	1.79	0.48
3:D:239:LEU:HD22	3:D:242:TYR:HE2	1.78	0.48
3:D:264:ILE:HG12	3:D:318:LEU:HB2	1.95	0.48
3:D:353:GLN:HG2	3:D:367:LEU:HD21	1.94	0.48
1:A:1255:VAL:HG12	1:A:1612:ILE:HG23	1.95	0.48
2:B:667:CYS:HA	2:B:697:CYS:CB	2.44	0.48
1:A:89:LYS:HA	1:A:92:THR:OG1	2.14	0.48
3:D:247:MET:HE3	3:D:359:ARG:HD3	1.96	0.48
3:D:353:GLN:HG2	3:D:367:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:TRP:N	1:A:1368:PRO:HD2	2.28	0.48
2:B:37:VAL:HG21	2:B:1006:GLU:HB3	1.94	0.48
2:B:987:SER:HB3	2:B:990:PHE:CZ	2.48	0.48
1:A:392:ILE:HD11	3:D:355:LEU:HD21	1.95	0.47
2:B:716:VAL:HG23	2:B:720:TRP:HE3	1.79	0.47
2:B:261:SER:O	2:B:327:ALA:HB1	2.14	0.47
1:A:108:ASN:HD21	1:A:198:ARG:HH11	1.62	0.47
1:A:1396:TYR:O	1:A:1400:PHE:HD2	1.97	0.47
1:A:388:TYR:CE1	3:D:392:ASN:HA	2.48	0.47
1:A:1258:PRO:O	1:A:1261:THR:HG22	2.14	0.47
1:A:1481:ILE:O	1:A:1485:THR:HG23	2.15	0.47
1:A:1538:PHE:O	1:A:1542:THR:HG23	2.14	0.47
2:B:109:ALA:HB2	2:B:469:ILE:HG23	1.95	0.47
1:A:1255:VAL:O	1:A:1258:PRO:HD2	2.14	0.47
1:A:584:ARG:NH2	8:A:2419:PT5:O53	2.44	0.47
2:B:481:ASN:OD1	4:E:1:NAG:O6	2.28	0.47
2:B:147:PRO:HB3	2:B:163:HIS:NE2	2.29	0.47
6:A:2402:R16:H372	6:A:2402:R16:H341	1.68	0.47
1:A:591:TYR:HB3	1:A:1284:ASN:ND2	2.31	0.47
2:B:295:ASN:ND2	2:B:328:LYS:O	2.30	0.47
1:A:157:HIS:C	1:A:159:GLY:H	2.23	0.46
2:B:396:ARG:O	2:B:400:GLN:HG3	2.15	0.46
3:D:368:ASN:OD1	3:D:369:VAL:N	2.45	0.46
1:A:1247:ILE:O	1:A:1251:ARG:HG2	2.14	0.46
2:B:224:VAL:HG23	2:B:225:ASP:N	2.30	0.46
1:A:599:VAL:HG11	8:A:2419:PT5:H15	1.97	0.46
2:B:157:ARG:NH2	2:B:222:PRO:O	2.49	0.46
2:B:218:TYR:HB3	2:B:219:PRO:HD3	1.97	0.46
2:B:352:ALA:O	2:B:354:CYS:N	2.49	0.46
2:B:280:LEU:HA	2:B:283:LEU:HD12	1.97	0.46
2:B:508:PRO:HG3	2:B:759:TYR:CD1	2.50	0.46
3:D:332:LEU:HD23	3:D:332:LEU:O	2.15	0.46
1:A:1481:ILE:HD13	1:A:1514:PHE:CZ	2.51	0.46
2:B:114:ARG:NH1	2:B:116:ASP:O	2.49	0.46
1:A:679:VAL:HG22	1:A:683:MET:HE1	1.83	0.46
2:B:710:GLY:O	2:B:714:GLU:HG3	2.15	0.46
2:B:193:PHE:HB3	2:B:218:TYR:CG	2.51	0.46
3:D:348:SER:O	3:D:351:VAL:HG22	2.16	0.45
1:A:546:PHE:HZ	1:A:581:ARG:HA	1.81	0.45
1:A:1173:VAL:HG13	1:A:1174:ARG:HG3	1.98	0.45
1:A:1628:ASP:OD2	1:A:1634:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:667:CYS:HA	2:B:697:CYS:HB2	1.98	0.45
1:A:395:ALA:HB2	3:D:251:ALA:HB2	1.97	0.45
1:A:465:ARG:O	1:A:468:GLU:HG3	2.16	0.45
2:B:596:ASP:OD1	2:B:596:ASP:N	2.50	0.45
2:B:881:SER:OG	2:B:1026:CYS:O	2.34	0.45
1:A:307:VAL:O	1:A:311:ILE:HG12	2.17	0.45
1:A:683:MET:HB3	6:A:2407:R16:H332	1.99	0.45
1:A:1717:ASP:OD1	1:A:1718:SER:N	2.50	0.45
7:A:2409:Y01:HAE2	6:A:2410:R16:H322	1.98	0.45
1:A:1219:TRP:HE1	1:A:1269:LYS:HE3	1.82	0.45
1:A:299:ASN:OD1	1:A:300:ILE:N	2.47	0.45
1:A:1402:VAL:O	1:A:1406:PHE:HB3	2.17	0.45
2:B:50:THR:O	2:B:719:TYR:OH	2.29	0.45
1:A:1595:SER:CB	1:A:1710:ASN:HD21	2.30	0.45
1:A:1297:ALA:O	1:A:1301:VAL:HG23	2.17	0.45
1:A:252:ALA:HB2	1:A:287:TRP:CE3	2.52	0.44
1:A:377:ARG:HA	1:A:377:ARG:HD2	1.84	0.44
1:A:673:ILE:HD11	1:A:686:SER:HB3	2.00	0.44
2:B:398:PRO:O	2:B:402:MET:HG3	2.17	0.44
2:B:423:THR:CG2	2:B:426:TYR:HE2	2.28	0.44
2:B:860:LEU:HD12	2:B:860:LEU:HA	1.87	0.44
2:B:1001:ARG:HE	2:B:1020:SER:HB3	1.82	0.44
1:A:660:LEU:HD22	1:A:696:GLY:HA3	1.97	0.44
2:B:569:ASP:O	2:B:573:GLU:HG3	2.17	0.44
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.72	0.44
1:A:337:ILE:HD13	6:A:2414:R16:H301	1.98	0.44
2:B:112:GLN:OE1	2:B:112:GLN:N	2.46	0.44
2:B:1007:LYS:HA	2:B:1014:ILE:HA	1.99	0.44
1:A:1405:PHE:O	1:A:1409:ASN:ND2	2.48	0.44
1:A:1519:VAL:O	1:A:1522:ILE:HG22	2.18	0.44
2:B:660:PHE:HB2	2:B:741:THR:CG2	2.48	0.44
2:B:735:VAL:HG22	2:B:741:THR:OG1	2.17	0.44
1:A:181:THR:O	1:A:181:THR:HG22	2.18	0.44
1:A:720:LYS:HD2	1:A:769:GLU:OE2	2.18	0.44
2:B:494:LEU:HD12	2:B:494:LEU:HA	1.85	0.44
1:A:108:ASN:HD21	1:A:198:ARG:NH1	2.16	0.44
1:A:640:GLU:HG2	1:A:641:THR:N	2.33	0.44
1:A:1721:LEU:H	1:A:1721:LEU:HD23	1.83	0.44
1:A:616:LEU:O	1:A:620:ILE:HG13	2.18	0.43
2:B:780:PHE:CE1	2:B:870:GLN:HA	2.53	0.43
2:B:828:THR:HG22	2:B:831:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:271:ALA:HB3	3:D:305:GLU:OE2	2.18	0.43
1:A:154:PHE:HD1	1:A:155:VAL:HG13	1.83	0.43
1:A:399:MET:HG2	1:A:403:GLU:OE1	2.18	0.43
2:B:753:GLN:NE2	2:B:785:PRO:HG2	2.33	0.43
2:B:1039:ASP:OD1	2:B:1040:GLY:N	2.51	0.43
3:D:255:PHE:CE2	3:D:398:CYS:HB3	2.53	0.43
1:A:1519:VAL:O	1:A:1523:ILE:HG12	2.18	0.43
6:A:2401:R16:H411	6:A:2401:R16:H382	1.80	0.43
1:A:1289:TYR:CE1	1:A:1403:PHE:HD2	2.35	0.43
1:A:1496:PRO:O	1:A:1497:TYR:HB3	2.18	0.43
2:B:882:LEU:HD21	2:B:1016:ILE:HG21	2.00	0.43
1:A:496:THR:HA	1:A:499:VAL:HG22	1.99	0.43
1:A:657:PHE:O	1:A:661:THR:HG23	2.18	0.43
1:A:1359:PHE:O	1:A:1363:THR:HG23	2.18	0.43
7:A:2403:Y01:HAO2	7:A:2403:Y01:HAP1	1.27	0.43
2:B:432:ARG:HB2	2:B:433:PRO:HD3	2.01	0.43
2:B:470:THR:HG21	4:E:1:NAG:H5	2.00	0.43
2:B:635:LEU:HD23	2:B:635:LEU:HA	1.87	0.43
2:B:798:VAL:HG23	2:B:809:PRO:HD2	2.00	0.43
1:A:119:PRO:HG3	1:A:636:ASN:OD1	2.19	0.43
1:A:391:TRP:NE1	3:D:394:LEU:HD13	2.33	0.43
1:A:594:SER:HA	1:A:719:THR:HG21	2.00	0.43
1:A:1609:LEU:HD22	1:A:1698:LEU:HD22	2.00	0.43
2:B:392:HIS:HE1	2:B:396:ARG:HE	1.67	0.43
2:B:745:PRO:C	2:B:747:GLU:H	2.27	0.43
1:A:679:VAL:HG22	1:A:683:MET:CE	2.45	0.43
1:A:112:LEU:HD21	1:A:195:ARG:NE	2.34	0.43
3:D:230:ARG:NH2	3:D:339:PRO:O	2.52	0.43
1:A:484:PHE:HA	1:A:487:VAL:HG12	2.00	0.43
2:B:892:TYR:HA	2:B:982:PHE:O	2.19	0.43
1:A:1369:MET:HE3	1:A:1373:HIS:HE1	1.84	0.42
6:A:2401:R16:H281	6:A:2415:R16:H321	2.01	0.42
2:B:994:LEU:HD22	2:B:1001:ARG:HD3	2.00	0.42
3:D:353:GLN:NE2	3:D:357:LYS:HE2	2.31	0.42
1:A:1457:ARG:HA	1:A:1462:TYR:HB2	2.01	0.42
1:A:1519:VAL:HA	1:A:1522:ILE:HG22	2.00	0.42
2:B:261:SER:O	2:B:264:VAL:HG22	2.19	0.42
1:A:1591:THR:HG22	1:A:1710:ASN:OD1	2.19	0.42
2:B:860:LEU:HD22	2:B:1013:LEU:HD21	2.02	0.42
3:D:387:ILE:HD11	3:D:404:TYR:CE1	2.54	0.42
2:B:208:PHE:HD1	2:B:488:MET:SD	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:SER:O	1:A:1519:VAL:HG23	2.20	0.42
1:A:1840:LEU:O	1:A:1844:HIS:N	2.48	0.42
2:B:37:VAL:HA	2:B:40:MET:HG2	2.01	0.42
2:B:537:PRO:HD3	2:B:974:CYS:HB3	2.00	0.42
3:D:354:ARG:HE	3:D:354:ARG:HB3	1.71	0.42
1:A:176:THR:CG2	1:A:194:VAL:HG11	2.50	0.42
2:B:241:ARG:HD2	2:B:241:ARG:HA	1.80	0.42
2:B:991:SER:HB3	2:B:1004:HIS:ND1	2.35	0.42
1:A:650:PRO:O	1:A:653:ILE:HG22	2.19	0.42
8:A:2419:PT5:H52	8:A:2419:PT5:H18	1.75	0.42
2:B:306:HIS:CG	2:B:349:VAL:HG11	2.54	0.42
1:A:229:LEU:HD22	1:A:1585:ILE:HD11	2.02	0.42
1:A:314:GLU:HG3	1:A:665:TRP:CD1	2.55	0.42
1:A:723:GLU:O	1:A:727:GLU:OE1	2.37	0.42
3:D:303:GLN:HA	3:D:306:ILE:HD13	2.01	0.42
1:A:495:ASN:C	1:A:495:ASN:HD22	2.27	0.42
1:A:712:LEU:HD12	1:A:1413:ALA:HB3	2.02	0.42
1:A:771:ARG:HA	1:A:771:ARG:HD2	1.87	0.42
3:D:236:GLY:N	3:D:237:PRO:HD2	2.35	0.42
1:A:132:ASP:O	1:A:135:PRO:HD2	2.20	0.42
1:A:176:THR:HG23	1:A:191:LEU:HD12	2.01	0.42
1:A:262:PRO:HG3	1:A:287:TRP:CD1	2.55	0.42
2:B:93:ARG:HB2	2:B:446:TRP:HH2	1.85	0.42
2:B:295:ASN:C	2:B:297:ASN:H	2.28	0.42
1:A:1156:ILE:HD13	1:A:1156:ILE:HA	1.93	0.41
1:A:1484:ASN:C	1:A:1484:ASN:HD22	2.27	0.41
7:A:2409:Y01:HAS2	7:A:2409:Y01:HAE1	1.87	0.41
2:B:52:SER:OG	2:B:814:ILE:HG12	2.20	0.41
2:B:258:VAL:HG12	2:B:260:VAL:HG13	2.01	0.41
2:B:645:SER:HB3	2:B:687:ILE:HG21	2.02	0.41
1:A:1388:TYR:O	1:A:1389:ARG:C	2.63	0.41
1:A:1646:MET:HB2	6:A:2414:R16:H341	2.01	0.41
2:B:671:LYS:HD3	2:B:671:LYS:HA	1.82	0.41
3:D:343:TYR:CE2	3:D:345:LYS:HD2	2.56	0.41
2:B:193:PHE:CG	2:B:218:TYR:HB2	2.55	0.41
2:B:396:ARG:HD3	2:B:410:TYR:OH	2.21	0.41
2:B:735:VAL:HB	2:B:811:VAL:HG12	2.02	0.41
3:D:306:ILE:H	3:D:306:ILE:HD12	1.85	0.41
3:D:396:ASP:O	3:D:399:GLU:HG3	2.21	0.41
1:A:1565:SER:HB3	1:A:1568:ARG:HH11	1.85	0.41
1:A:1672:GLU:OE1	1:A:1672:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:752:TRP:NE1	2:B:754:GLU:HB2	2.35	0.41
3:D:329:PRO:HG3	3:D:385:PHE:CZ	2.56	0.41
1:A:676:GLN:HB3	6:A:2406:R16:H382	2.01	0.41
2:B:33:ILE:HA	2:B:36:TRP:HB3	2.02	0.41
2:B:168:ILE:HG12	2:B:214:LEU:CD2	2.50	0.41
1:A:207:PRO:HA	1:A:210:GLN:HG3	2.03	0.41
1:A:165:GLY:HA3	6:A:2408:R16:H322	2.03	0.41
1:A:1222:LEU:HA	1:A:1225:ILE:HG12	2.03	0.41
2:B:472:GLN:O	2:B:473:PHE:HB2	2.21	0.41
1:A:340:ILE:O	1:A:344:SER:OG	2.31	0.41
1:A:591:TYR:HB3	1:A:1284:ASN:HD21	1.85	0.41
1:A:1487:VAL:HG21	1:A:1510:PHE:HE2	1.85	0.41
1:A:1721:LEU:HD22	1:A:1802:ALA:HB1	2.02	0.41
6:A:2417:R16:H311	6:A:2417:R16:H281	1.88	0.41
2:B:289:VAL:HG12	2:B:310:ALA:HB2	2.03	0.41
2:B:317:VAL:HG21	2:B:1043:PRO:HG2	2.03	0.41
2:B:856:GLY:HA2	2:B:981:TYR:HB2	2.02	0.41
1:A:108:ASN:HD21	1:A:198:ARG:HD3	1.85	0.41
1:A:1583:TYR:O	1:A:1587:ILE:HG12	2.21	0.41
1:A:1818:ASP:HA	1:A:1821:LEU:HD12	2.02	0.41
2:B:884:ARG:HH22	2:B:1029:ARG:C	2.29	0.41
1:A:493:ALA:HB2	1:A:582:LEU:HD21	2.03	0.40
1:A:1181:ASN:O	1:A:1184:LYS:HG2	2.21	0.40
2:B:653:PHE:CZ	2:B:659:THR:HB	2.56	0.40
2:B:1005:GLY:HA2	2:B:1015:PHE:O	2.20	0.40
1:A:295:THR:HA	1:A:306:THR:HG22	2.03	0.40
1:A:391:TRP:CD1	3:D:394:LEU:HD13	2.57	0.40
1:A:1179:ARG:NH2	7:A:2418:Y01:HBC	2.37	0.40
1:A:1369:MET:HE3	1:A:1373:HIS:CE1	2.55	0.40
2:B:186:THR:HG22	2:B:189:LEU:HD12	2.03	0.40
2:B:421:ILE:O	2:B:425:GLU:HG3	2.22	0.40
3:D:387:ILE:HD13	3:D:387:ILE:HA	1.88	0.40
1:A:1367:TRP:CD1	1:A:1368:PRO:HD3	2.57	0.40
1:A:1406:PHE:CD1	8:A:2419:PT5:H47	2.57	0.40
1:A:1305:LYS:HE2	1:A:1305:LYS:HB3	1.92	0.40
1:A:1473:PHE:O	1:A:1477:ILE:HG12	2.21	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%)	1192 (96%)	56 (4%)	0	100	100
2	B	947/1103 (86%)	898 (95%)	49 (5%)	0	100	100
3	D	158/598 (26%)	152 (96%)	6 (4%)	0	100	100
All	All	2353/4040 (58%)	2242 (95%)	111 (5%)	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%)	1089 (100%)	0	100	100
2	B	846/971 (87%)	846 (100%)	0	100	100
3	D	131/510 (26%)	131 (100%)	0	100	100
All	All	2066/3472 (60%)	2066 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	309	GLN
1	A	324	ASN

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Mol	Chain	Res	Type
1	A	332	ASN
1	A	495	ASN
1	A	697	ASN
1	A	778	GLN
1	A	1284	ASN
1	A	1559	ASN
1	A	1667	ASN
2	B	374	ASN
2	B	392	HIS
2	B	424	GLN
2	B	443	GLN
2	B	753	GLN
2	B	978	GLN
3	D	328	HIS
3	D	353	GLN
3	D	363	GLN
3	D	366	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	1	4,2	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	C	2	4	14,14,15	0.19	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	C	3	4	11,11,12	0.58	0	15,15,17	0.70	0
4	NAG	E	1	4,2	14,14,15	0.40	0	17,19,21	0.49	0
4	NAG	E	2	4	14,14,15	0.19	0	17,19,21	0.57	0
4	BMA	E	3	4	11,11,12	0.56	0	15,15,17	0.65	0
5	NAG	F	1	5,2	14,14,15	0.78	1 (7%)	17,19,21	1.01	1 (5%)
5	NAG	F	2	5	14,14,15	0.30	0	17,19,21	0.47	0
5	BMA	F	3	5	11,11,12	0.61	0	15,15,17	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	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)
5	F	1	NAG	O5-C1	2.59	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	3.89	117.40	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6

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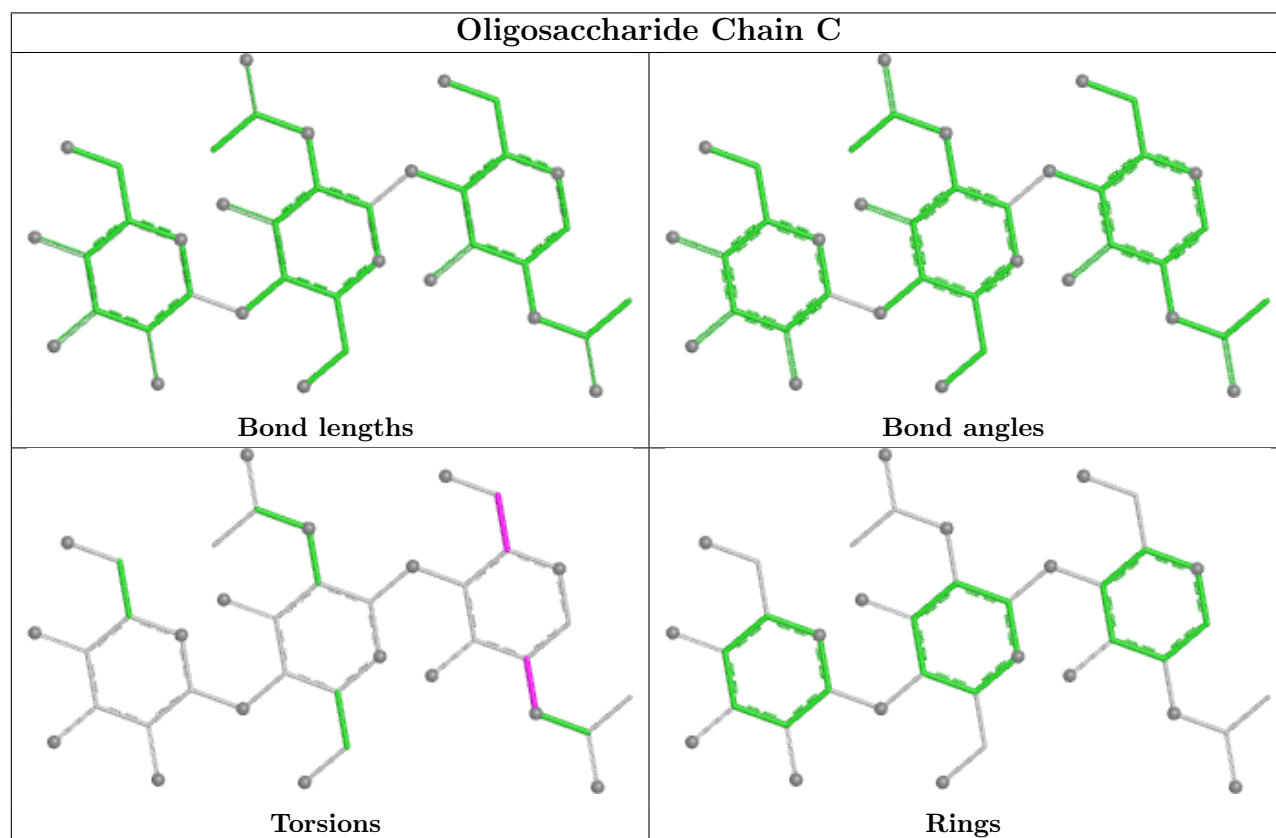
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	C	1	NAG	C1-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C1-C2-N2-C7
4	C	1	NAG	C3-C2-N2-C7

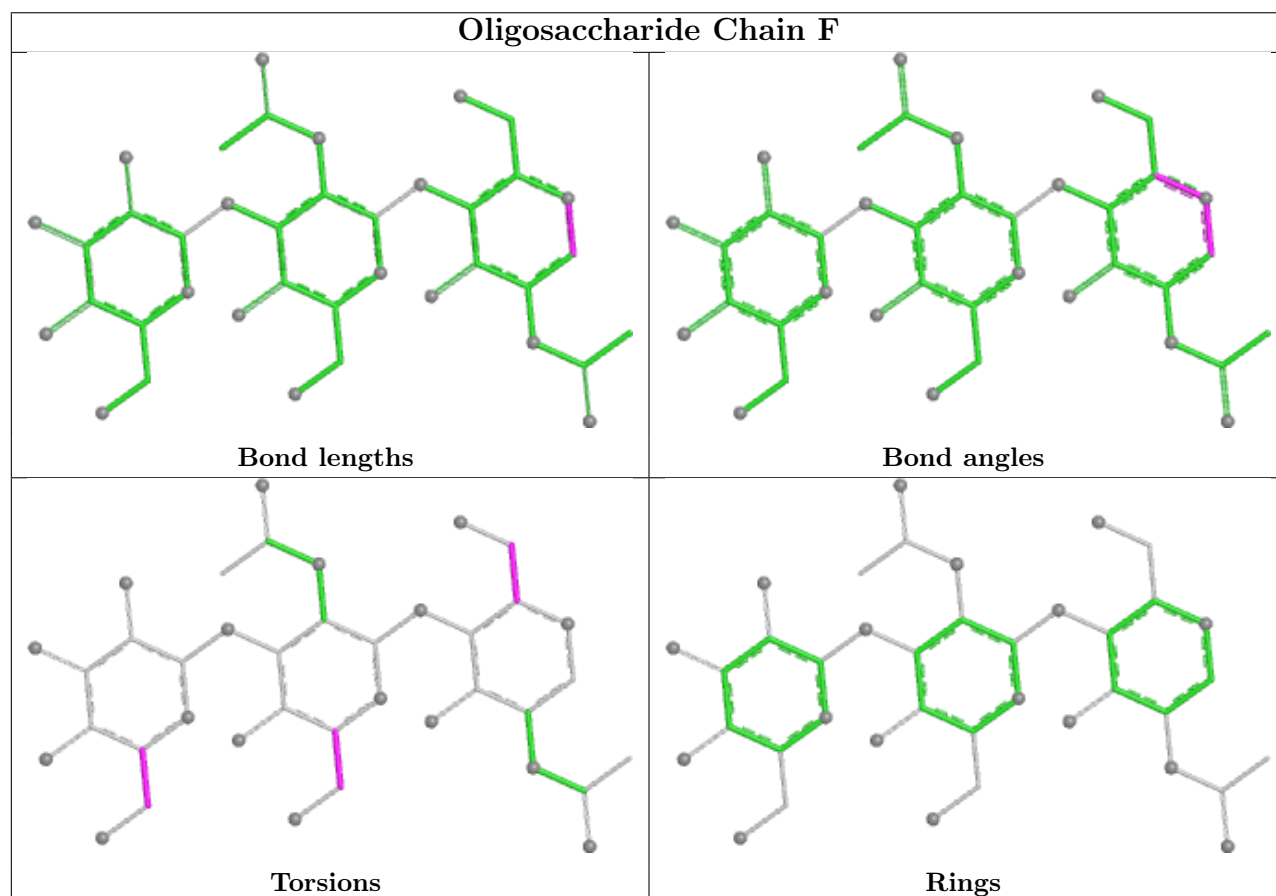
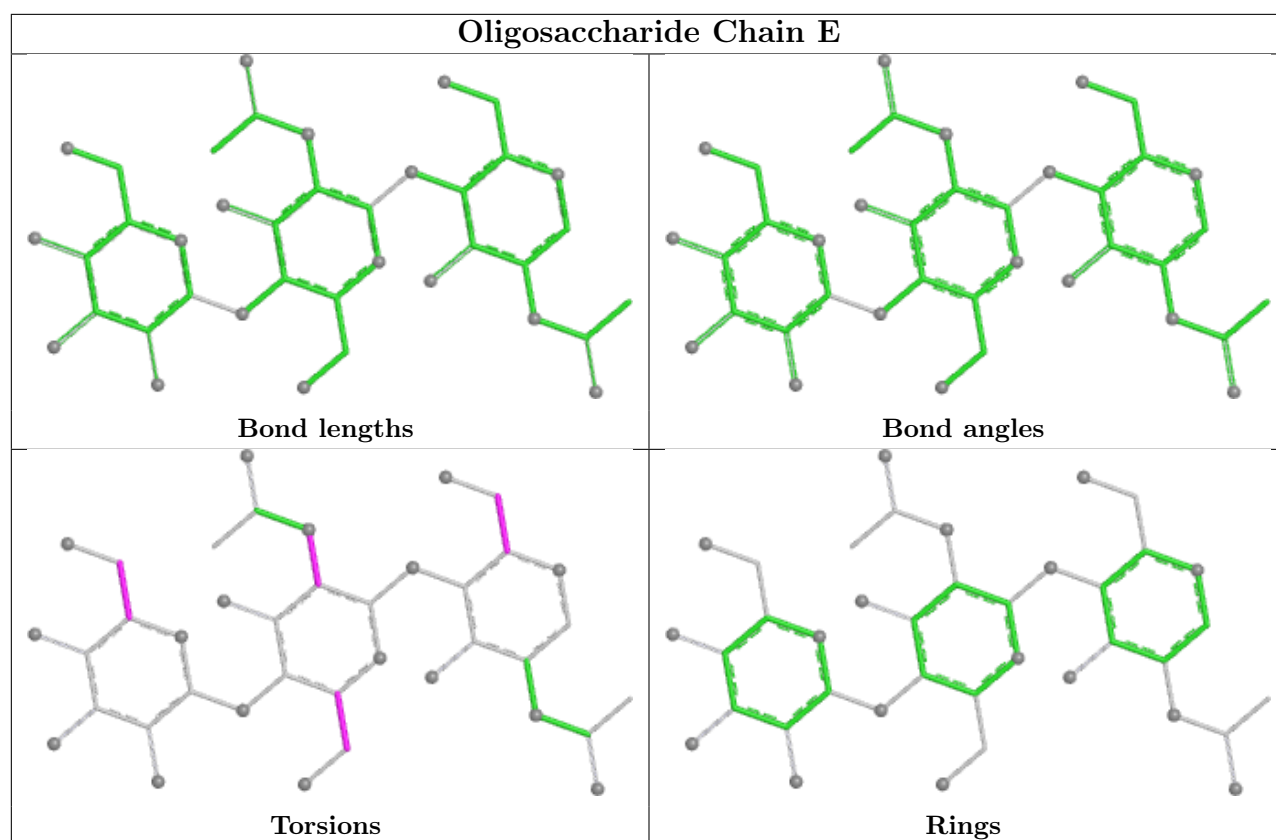
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	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

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	2	14,14,15	0.23	0	17,19,21	0.50	0
6	R16	A	2404	-	15,15,15	0.14	0	14,14,14	0.17	0
11	NAG	B	1203	2	14,14,15	0.27	0	17,19,21	0.47	0
11	NAG	B	1209	2	14,14,15	0.22	0	17,19,21	0.52	0
11	NAG	B	1206	2	14,14,15	0.18	0	17,19,21	0.42	0
6	R16	A	2414	-	14,14,15	0.13	0	13,13,14	0.26	0
6	R16	A	2412	-	12,12,15	0.13	0	11,11,14	0.21	0
6	R16	A	2417	-	15,15,15	0.12	0	14,14,14	0.08	0
8	PT5	A	2419	-	62,62,69	1.49	10 (16%)	77,80,87	0.98	3 (3%)
11	NAG	B	1204	2	14,14,15	0.25	0	17,19,21	0.58	0
6	R16	A	2405	-	15,15,15	0.16	0	14,14,14	0.17	0
6	R16	A	2410	-	12,12,15	0.12	0	11,11,14	0.19	0
7	Y01	A	2409	-	38,38,38	4.20	12 (31%)	57,57,57	2.17	18 (31%)
7	Y01	A	2403	-	38,38,38	0.59	0	57,57,57	0.89	3 (5%)
11	NAG	B	1205	2	14,14,15	0.36	0	17,19,21	0.50	0
6	R16	A	2408	-	10,10,15	0.17	0	9,9,14	0.09	0
6	R16	A	2402	-	15,15,15	0.16	0	14,14,14	0.07	0
11	NAG	B	1207	2	14,14,15	0.20	0	17,19,21	0.42	0
6	R16	A	2416	-	15,15,15	0.16	0	14,14,14	0.19	0
11	NAG	B	1208	2	14,14,15	0.26	0	17,19,21	0.57	0
6	R16	A	2411	-	14,14,15	0.14	0	13,13,14	0.18	0
6	R16	A	2415	-	12,12,15	0.24	0	11,11,14	0.09	0
6	R16	A	2407	-	15,15,15	0.13	0	14,14,14	0.21	0
6	R16	A	2413	-	11,11,15	0.12	0	10,10,14	0.20	0
9	6I7	A	2420	-	33,33,33	2.05	9 (27%)	47,50,50	3.13	13 (27%)
6	R16	A	2406	-	15,15,15	0.13	0	14,14,14	0.14	0
6	R16	A	2401	-	15,15,15	0.14	0	14,14,14	0.20	0
7	Y01	A	2418	-	38,38,38	0.50	0	57,57,57	0.96	2 (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
11	NAG	B	1202	2	-	2/6/23/26	0/1/1/1
6	R16	A	2404	-	-	6/13/13/13	-
11	NAG	B	1203	2	-	0/6/23/26	0/1/1/1
11	NAG	B	1209	2	-	0/6/23/26	0/1/1/1
11	NAG	B	1206	2	-	2/6/23/26	0/1/1/1
6	R16	A	2414	-	-	4/12/12/13	-
6	R16	A	2412	-	-	1/10/10/13	-
6	R16	A	2417	-	-	10/13/13/13	-
8	PT5	A	2419	-	-	24/59/83/90	0/1/1/1
11	NAG	B	1204	2	-	4/6/23/26	0/1/1/1
6	R16	A	2405	-	-	6/13/13/13	-
6	R16	A	2410	-	-	5/10/10/13	-
7	Y01	A	2409	-	-	9/19/77/77	0/4/4/4
7	Y01	A	2403	-	-	10/19/77/77	0/4/4/4
11	NAG	B	1205	2	-	2/6/23/26	0/1/1/1
6	R16	A	2408	-	-	5/8/8/13	-
6	R16	A	2402	-	-	7/13/13/13	-
11	NAG	B	1207	2	-	0/6/23/26	0/1/1/1
6	R16	A	2416	-	-	7/13/13/13	-
11	NAG	B	1208	2	-	4/6/23/26	0/1/1/1
6	R16	A	2411	-	-	4/12/12/13	-
6	R16	A	2415	-	-	5/10/10/13	-
6	R16	A	2407	-	-	6/13/13/13	-
6	R16	A	2413	-	-	4/9/9/13	-
9	6I7	A	2420	-	-	1/14/30/30	0/4/4/4
6	R16	A	2406	-	-	3/13/13/13	-
6	R16	A	2401	-	-	5/13/13/13	-
7	Y01	A	2418	-	-	10/19/77/77	0/4/4/4

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2409	Y01	CAI-CAZ	17.43	1.69	1.33
7	A	2409	Y01	CBH-CBF	7.30	1.67	1.56
7	A	2409	Y01	CAU-CBI	-7.20	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2409	Y01	CAQ-CAP	6.88	1.72	1.54
9	A	2420	6I7	C20-C19	6.45	1.56	1.49
7	A	2409	Y01	CAK-CBD	6.30	1.63	1.53
7	A	2409	Y01	CAU-CAS	6.29	1.65	1.53
7	A	2409	Y01	CBI-CBE	5.70	1.65	1.55
7	A	2409	Y01	CBB-CBE	-5.27	1.45	1.54
7	A	2409	Y01	CAQ-CBG	5.17	1.64	1.54
9	A	2420	6I7	C10-N09	-4.86	1.32	1.37
9	A	2420	6I7	C11-C10	4.66	1.55	1.48
8	A	2419	PT5	C19-C18	4.02	1.54	1.31
8	A	2419	PT5	C16-C15	3.94	1.54	1.31
8	A	2419	PT5	C22-C21	3.90	1.53	1.31
8	A	2419	PT5	C25-C24	3.79	1.53	1.31
8	A	2419	PT5	P4-O4	3.57	1.65	1.59
8	A	2419	PT5	P5-O5	3.49	1.65	1.59
9	A	2420	6I7	O02-C03	3.40	1.42	1.37
7	A	2409	Y01	OAW-CAY	3.00	1.42	1.34
7	A	2409	Y01	CAO-CBB	2.86	1.61	1.54
8	A	2419	PT5	O18-C11	2.75	1.41	1.33
7	A	2409	Y01	CBH-CAZ	-2.61	1.47	1.52
8	A	2419	PT5	O16-C10	2.47	1.41	1.34
9	A	2420	6I7	C08-N09	2.29	1.46	1.43
8	A	2419	PT5	O16-C8	-2.27	1.41	1.46
8	A	2419	PT5	P1-O1	2.25	1.66	1.59
9	A	2420	6I7	C29-C20	-2.24	1.48	1.53
9	A	2420	6I7	C14-CL1	2.15	1.79	1.74
9	A	2420	6I7	C28-C26	2.14	1.57	1.52
9	A	2420	6I7	C21-C20	-2.00	1.48	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2420	6I7	C29-C20-C19	-13.89	83.04	112.00
9	A	2420	6I7	C21-C20-C19	11.08	135.10	112.00
7	A	2409	Y01	CAK-CAI-CAZ	-5.69	115.42	125.02
7	A	2409	Y01	CAD-CBH-CBF	-4.87	106.19	111.66
7	A	2409	Y01	CAU-CBI-CBE	4.72	123.55	116.60
9	A	2420	6I7	O25-C26-C29	4.21	116.88	110.47
9	A	2420	6I7	C18-C19-N30	-4.21	106.57	111.42
7	A	2409	Y01	CBH-CAZ-CAI	-4.17	116.84	122.93
7	A	2409	Y01	OAW-CAY-CAM	4.15	120.46	111.48
8	A	2419	PT5	O16-C10-C12	4.06	120.27	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2409	Y01	CAE-CBI-CBG	-3.85	104.70	111.68
9	A	2420	6I7	C10-N09-N30	-3.82	109.77	112.19
7	A	2409	Y01	CBI-CBE-CBB	-3.52	114.06	119.50
9	A	2420	6I7	C20-C19-C18	3.50	133.09	128.60
7	A	2409	Y01	CAE-CBI-CBE	-3.50	105.34	111.68
7	A	2409	Y01	CAT-CAR-CBC	3.48	116.00	110.33
7	A	2409	Y01	CBG-CBI-CBE	3.45	104.06	100.10
9	A	2420	6I7	C22-O25-C26	-3.37	117.04	122.03
9	A	2420	6I7	O02-C03-C08	3.24	120.06	116.04
9	A	2420	6I7	C10-C18-C19	3.21	107.69	104.08
7	A	2409	Y01	CAE-CBI-CAU	-3.20	105.89	110.61
7	A	2409	Y01	CBF-CBD-CBG	3.14	113.18	109.09
7	A	2409	Y01	CAU-CBI-CBG	3.01	111.75	107.25
8	A	2419	PT5	O18-C11-C31	2.72	120.12	111.83
7	A	2418	Y01	CAT-CAR-CBC	2.68	114.70	110.33
7	A	2403	Y01	CBG-CBI-CBE	2.57	103.04	100.10
7	A	2409	Y01	CAC-CBB-CBE	-2.53	109.09	112.88
9	A	2420	6I7	C01-O02-C03	-2.51	113.83	117.51
7	A	2409	Y01	CBF-CBH-CAZ	2.50	113.31	109.65
9	A	2420	6I7	O02-C03-C04	-2.48	120.12	124.30
9	A	2420	6I7	C08-N09-N30	2.35	122.36	118.74
8	A	2419	PT5	P4-O4-C4	-2.26	117.41	123.43
7	A	2409	Y01	CAO-CBB-CBE	2.23	114.96	110.33
9	A	2420	6I7	C29-C20-C21	2.22	117.08	109.44
7	A	2403	Y01	CAP-CAQ-CBG	-2.13	100.97	105.14
7	A	2409	Y01	CAV-CAZ-CBH	-2.11	113.72	116.42
7	A	2409	Y01	CAK-CBD-CBG	-2.05	108.03	110.93
7	A	2403	Y01	CAU-CBI-CBG	-2.03	104.20	107.25
7	A	2418	Y01	CBG-CBI-CBE	2.01	102.41	100.10

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2403	Y01	CAO-CBB-CBE-CAP
7	A	2403	Y01	CAO-CBB-CBE-CBI
7	A	2403	Y01	CAC-CBB-CBE-CBI
7	A	2418	Y01	OAG-CAY-OAW-CBC
7	A	2418	Y01	CAM-CAY-OAW-CBC
8	A	2419	PT5	C7-O13-P1-O12
8	A	2419	PT5	C7-O13-P1-O11
8	A	2419	PT5	C7-O13-P1-O1

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Mol	Chain	Res	Type	Atoms
8	A	2419	PT5	C12-C10-O16-C8
8	A	2419	PT5	O19-C11-O18-C9
8	A	2419	PT5	C31-C11-O18-C9
7	A	2403	Y01	CAC-CBB-CBE-CAP
8	A	2419	PT5	O17-C10-O16-C8
7	A	2418	Y01	CAJ-CAO-CBB-CAC
7	A	2409	Y01	CAX-CAL-CAM-CAY
11	B	1208	NAG	O5-C5-C6-O6
11	B	1206	NAG	O5-C5-C6-O6
11	B	1202	NAG	O5-C5-C6-O6
11	B	1204	NAG	O5-C5-C6-O6
11	B	1205	NAG	O5-C5-C6-O6
11	B	1208	NAG	C4-C5-C6-O6
11	B	1205	NAG	C4-C5-C6-O6
7	A	2403	Y01	CAJ-CAO-CBB-CAC
8	A	2419	PT5	C14-C15-C16-C17
11	B	1202	NAG	C4-C5-C6-O6
6	A	2417	R16	C28-C29-C30-C31
11	B	1204	NAG	C4-C5-C6-O6
11	B	1206	NAG	C4-C5-C6-O6
6	A	2402	R16	C32-C33-C34-C35
8	A	2419	PT5	C17-C18-C19-C20
7	A	2418	Y01	CAN-CAJ-CAO-CBB
7	A	2418	Y01	CAJ-CAN-CBA-CAB
6	A	2417	R16	C36-C37-C38-C39
6	A	2401	R16	C28-C29-C30-C31
6	A	2405	R16	C28-C29-C30-C31
6	A	2415	R16	C35-C36-C37-C38
7	A	2409	Y01	CAJ-CAN-CBA-CAB
6	A	2417	R16	C35-C36-C37-C38
7	A	2403	Y01	CAM-CAY-OAW-CBC
6	A	2407	R16	C33-C34-C35-C36
6	A	2413	R16	C35-C36-C37-C38
7	A	2409	Y01	CAJ-CAN-CBA-CAA
6	A	2408	R16	C35-C36-C37-C38
6	A	2406	R16	C34-C35-C36-C37
6	A	2411	R16	C31-C32-C33-C34
6	A	2411	R16	C28-C29-C30-C31
6	A	2416	R16	C37-C38-C39-C40
7	A	2418	Y01	CAJ-CAN-CBA-CAA
8	A	2419	PT5	C20-C21-C22-C23
6	A	2408	R16	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
7	A	2409	Y01	CAC-CBB-CBE-CBI
6	A	2405	R16	C33-C34-C35-C36
6	A	2408	R16	C36-C37-C38-C39
8	A	2419	PT5	C36-C37-C38-C39
6	A	2411	R16	C37-C38-C39-C40
8	A	2419	PT5	C31-C32-C33-C34
6	A	2417	R16	C37-C38-C39-C40
7	A	2403	Y01	OAG-CAY-OAW-CBC
7	A	2409	Y01	CAO-CBB-CBE-CBI
6	A	2414	R16	C35-C36-C37-C38
7	A	2403	Y01	CAO-CAJ-CAN-CBA
6	A	2410	R16	C37-C38-C39-C40
6	A	2401	R16	C37-C38-C39-C40
6	A	2417	R16	C33-C34-C35-C36
8	A	2419	PT5	C27-C28-C29-C30
7	A	2418	Y01	CAX-CAL-CAM-CAY
7	A	2409	Y01	CAJ-CAO-CBB-CBE
6	A	2408	R16	C33-C34-C35-C36
6	A	2414	R16	C37-C38-C39-C40
9	A	2420	6I7	N30-C19-C20-C29
7	A	2418	Y01	CAJ-CAO-CBB-CBE
6	A	2402	R16	C34-C35-C36-C37
6	A	2413	R16	C34-C35-C36-C37
6	A	2415	R16	C38-C39-C40-C41
6	A	2410	R16	C34-C35-C36-C37
6	A	2405	R16	C29-C30-C31-C32
8	A	2419	PT5	C25-C26-C27-C28
6	A	2415	R16	C33-C34-C35-C36
6	A	2413	R16	C36-C37-C38-C39
6	A	2404	R16	C32-C33-C34-C35
6	A	2407	R16	C32-C33-C34-C35
6	A	2416	R16	C27-C28-C29-C30
6	A	2404	R16	C28-C29-C30-C31
6	A	2407	R16	C29-C30-C31-C32
6	A	2402	R16	C35-C36-C37-C38
6	A	2416	R16	C28-C29-C30-C31
6	A	2404	R16	C38-C39-C40-C41
6	A	2416	R16	C32-C33-C34-C35
6	A	2415	R16	C39-C40-C41-C42
7	A	2409	Y01	CAC-CBB-CBE-CAP
8	A	2419	PT5	O13-C7-C8-O16
8	A	2419	PT5	C8-C7-O13-P1

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Mol	Chain	Res	Type	Atoms
6	A	2402	R16	C28-C29-C30-C31
6	A	2401	R16	C34-C35-C36-C37
11	B	1204	NAG	C1-C2-N2-C7
11	B	1208	NAG	C1-C2-N2-C7
6	A	2417	R16	C31-C32-C33-C34
6	A	2405	R16	C34-C35-C36-C37
6	A	2405	R16	C38-C39-C40-C41
6	A	2417	R16	C34-C35-C36-C37
6	A	2404	R16	C30-C31-C32-C33
6	A	2401	R16	C27-C28-C29-C30
6	A	2402	R16	C30-C31-C32-C33
6	A	2414	R16	C28-C29-C30-C31
6	A	2407	R16	C34-C35-C36-C37
6	A	2401	R16	C38-C39-C40-C41
11	B	1208	NAG	C3-C2-N2-C7
7	A	2409	Y01	CAO-CBB-CBE-CAP
6	A	2407	R16	C37-C38-C39-C40
8	A	2419	PT5	C9-C8-O16-C10
6	A	2405	R16	C35-C36-C37-C38
6	A	2406	R16	C30-C31-C32-C33
8	A	2419	PT5	C33-C34-C35-C36
6	A	2402	R16	C36-C37-C38-C39
6	A	2417	R16	C30-C31-C32-C33
8	A	2419	PT5	C37-C38-C39-C40
6	A	2413	R16	C37-C38-C39-C40
6	A	2412	R16	C33-C34-C35-C36
8	A	2419	PT5	C5-O5-P5-O51
6	A	2417	R16	C32-C33-C34-C35
7	A	2409	Y01	CAJ-CAO-CBB-CAC
6	A	2410	R16	C30-C31-C32-C33
6	A	2407	R16	C39-C40-C41-C42
6	A	2404	R16	C29-C30-C31-C32
6	A	2410	R16	C38-C39-C40-C41
6	A	2415	R16	C30-C31-C32-C33
8	A	2419	PT5	C15-C16-C17-C18
6	A	2416	R16	C34-C35-C36-C37
8	A	2419	PT5	C4-O4-P4-O42
8	A	2419	PT5	C5-O5-P5-O52
6	A	2411	R16	C36-C37-C38-C39
6	A	2417	R16	C39-C40-C41-C42
6	A	2416	R16	C39-C40-C41-C42
11	B	1204	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	A	2404	R16	C31-C32-C33-C34
8	A	2419	PT5	O13-C7-C8-C9
6	A	2416	R16	C36-C37-C38-C39
6	A	2408	R16	C32-C33-C34-C35
6	A	2410	R16	C32-C33-C34-C35
6	A	2406	R16	C35-C36-C37-C38
7	A	2403	Y01	CAL-CAM-CAY-OAW
7	A	2418	Y01	CAM-CAL-CAX-OAF
6	A	2414	R16	C29-C30-C31-C32
7	A	2418	Y01	CAM-CAL-CAX-OAH
6	A	2402	R16	C33-C34-C35-C36
7	A	2403	Y01	CAL-CAM-CAY-OAG

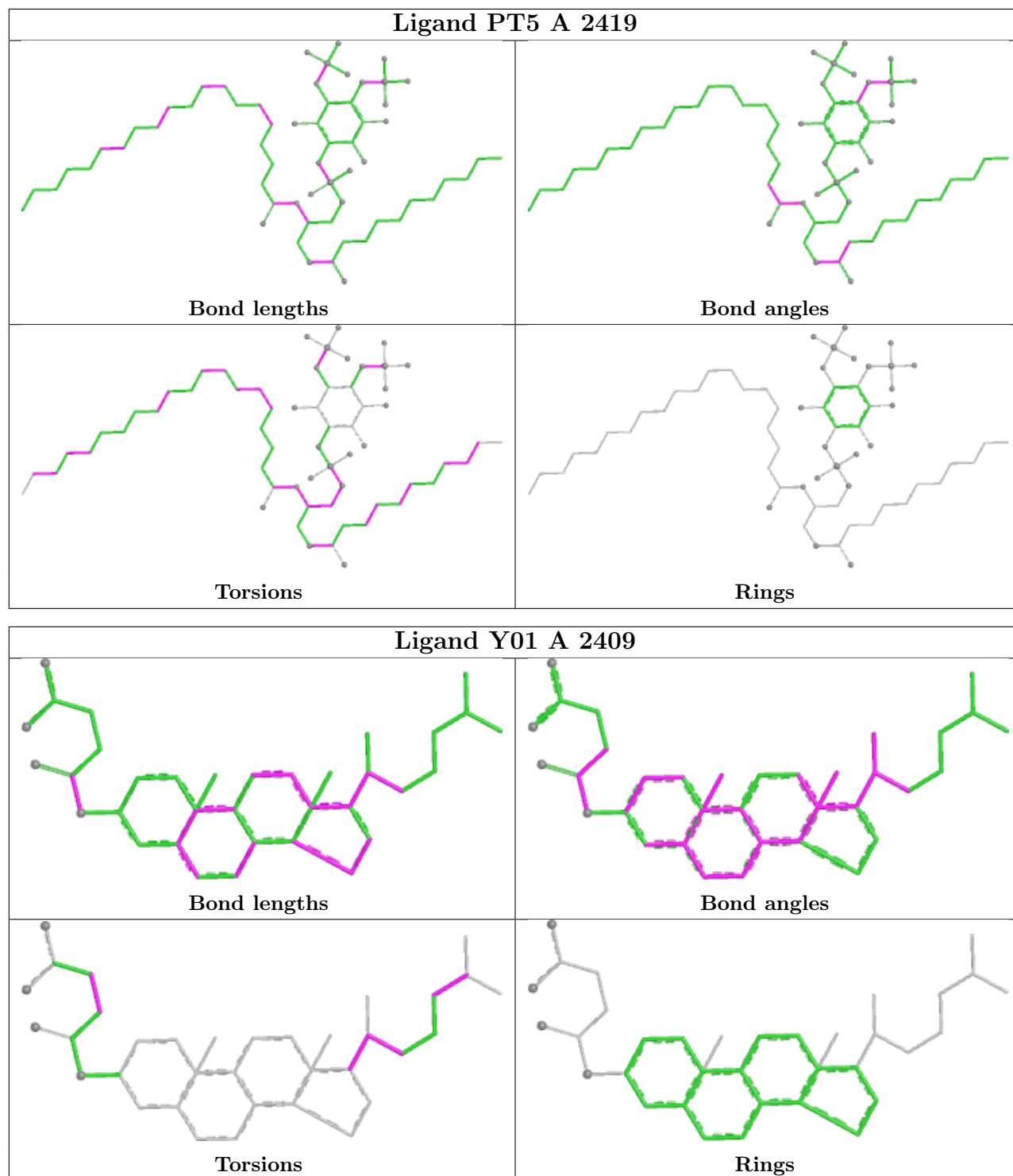
There are no ring outliers.

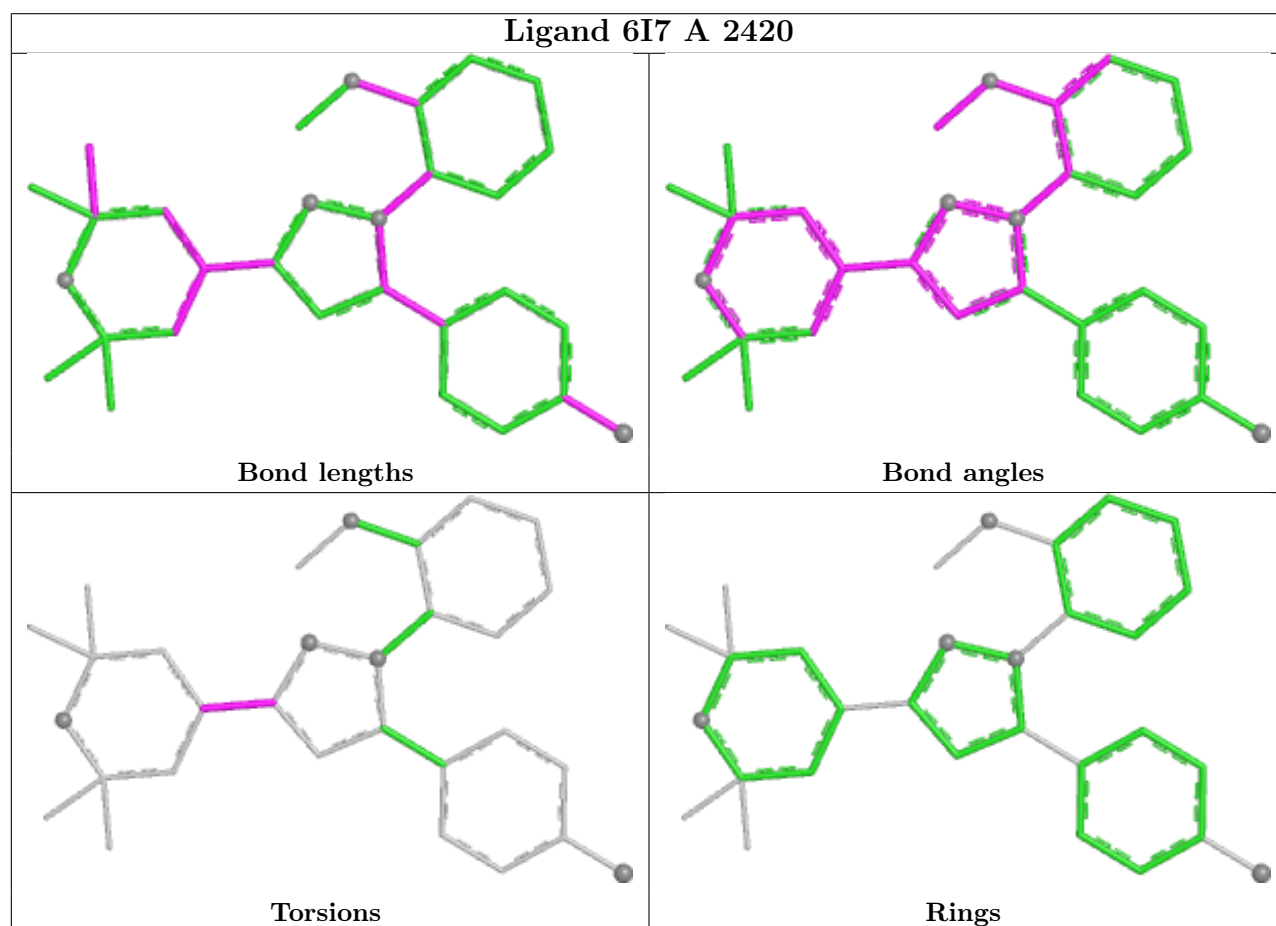
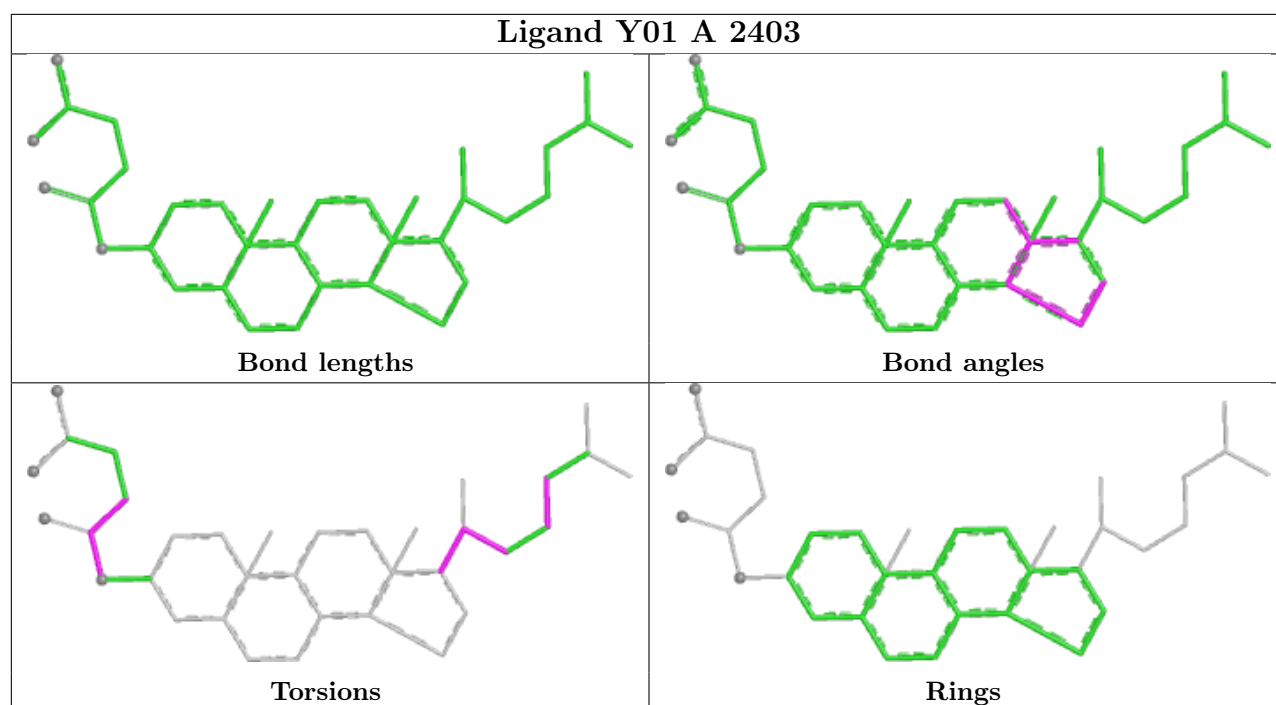
17 monomers are involved in 28 short contacts:

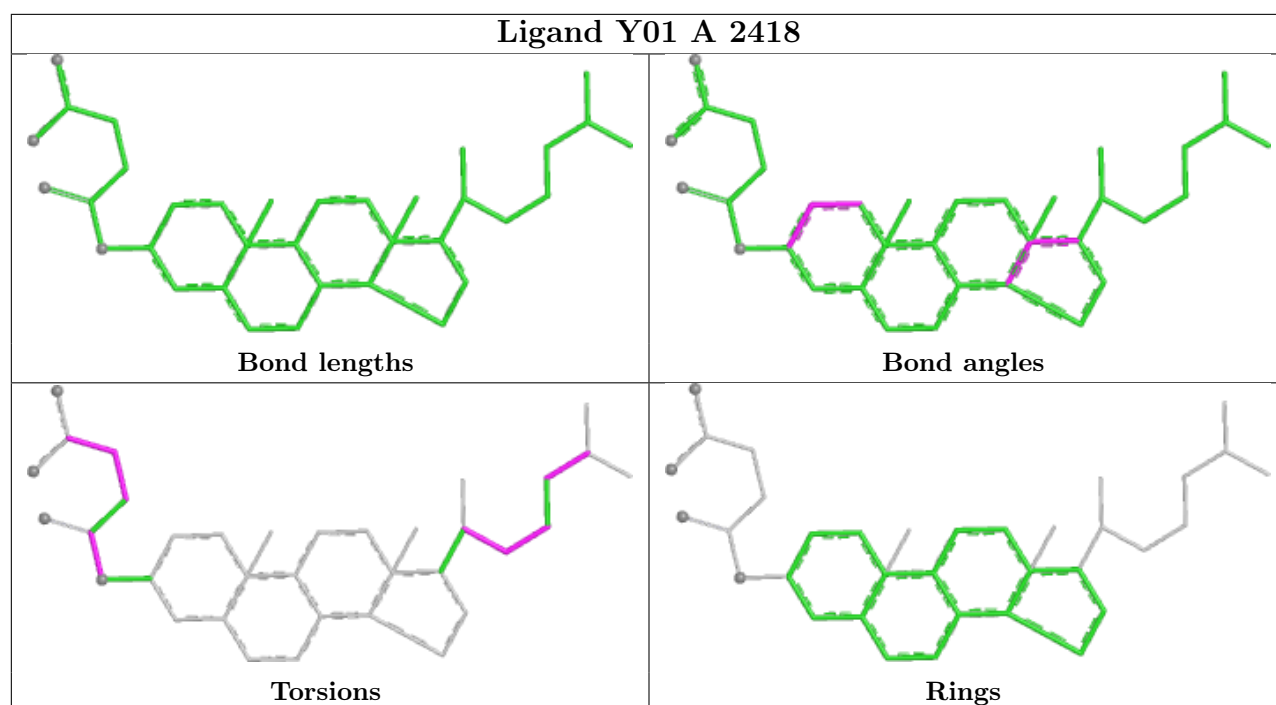
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1209	NAG	1	0
11	B	1206	NAG	1	0
6	A	2414	R16	2	0
6	A	2417	R16	1	0
8	A	2419	PT5	7	0
6	A	2410	R16	1	0
7	A	2409	Y01	3	0
7	A	2403	Y01	2	0
11	B	1205	NAG	1	0
6	A	2408	R16	1	0
6	A	2402	R16	1	0
6	A	2415	R16	1	0
6	A	2407	R16	2	0
9	A	2420	6I7	1	0
6	A	2406	R16	1	0
6	A	2401	R16	3	0
7	A	2418	Y01	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.

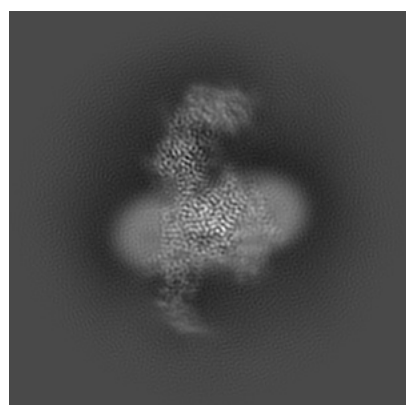
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31961. These allow visual inspection of the internal detail of the map and identification of artifacts.

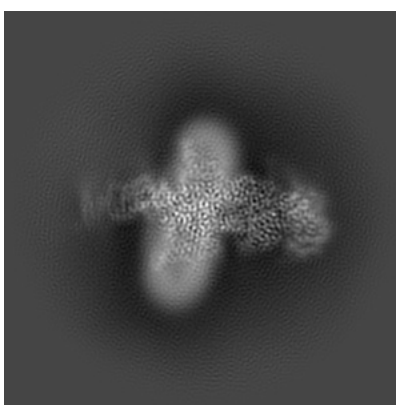
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

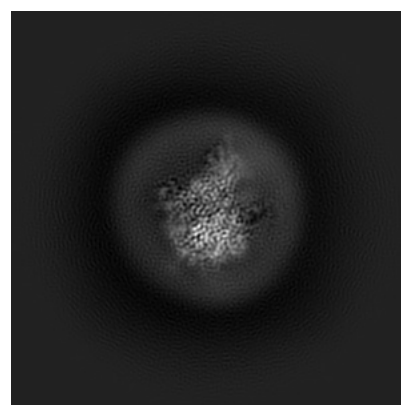
6.1.1 Primary map



X



Y

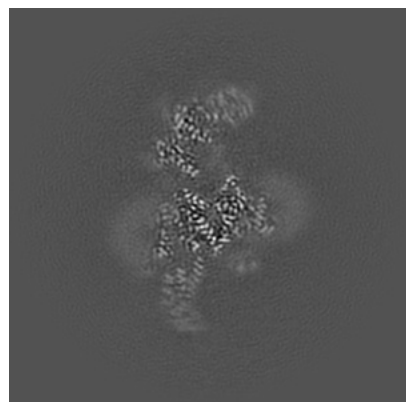


Z

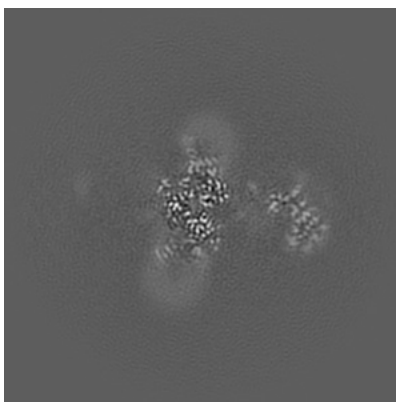
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

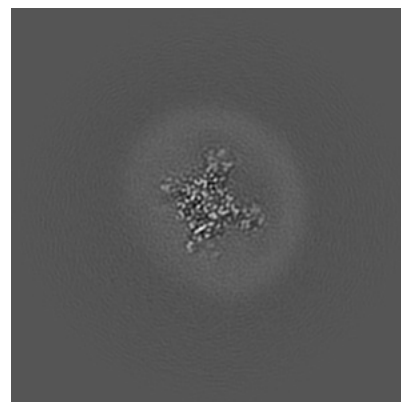
6.2.1 Primary map



X Index: 160



Y Index: 160

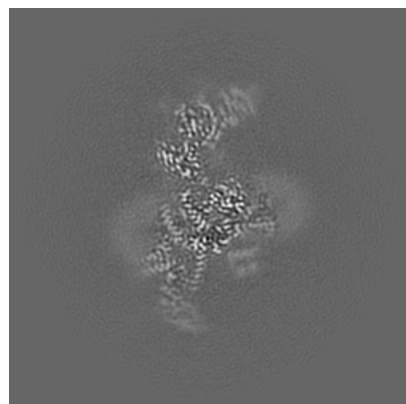


Z Index: 160

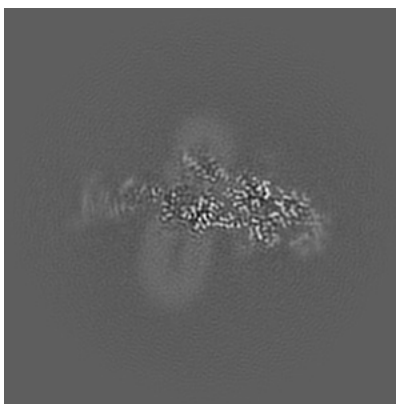
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

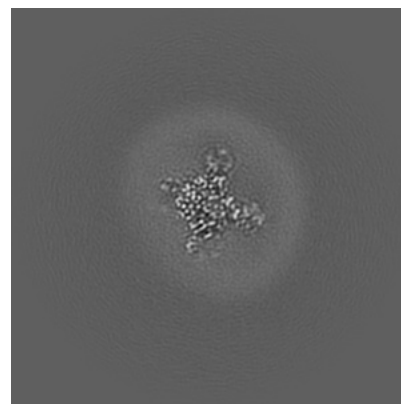
6.3.1 Primary map



X Index: 164



Y Index: 144

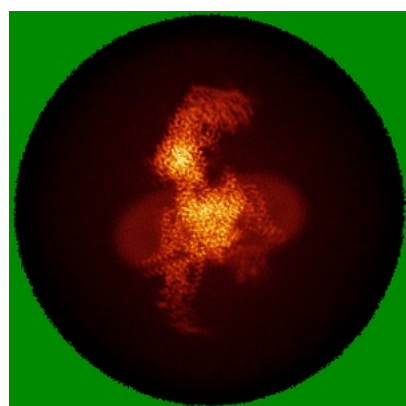


Z Index: 159

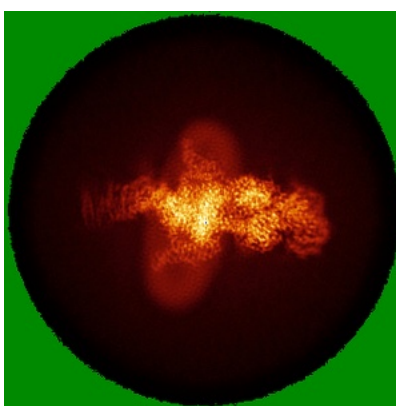
The images above show the largest variance slices of the map in three orthogonal directions.

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

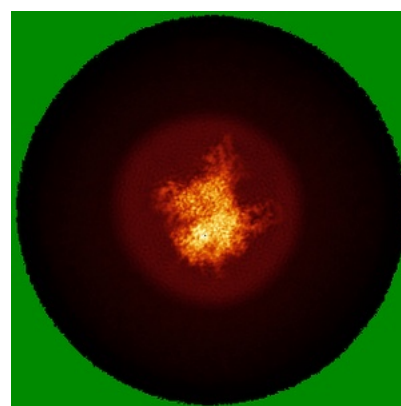
6.4.1 Primary map



X



Y

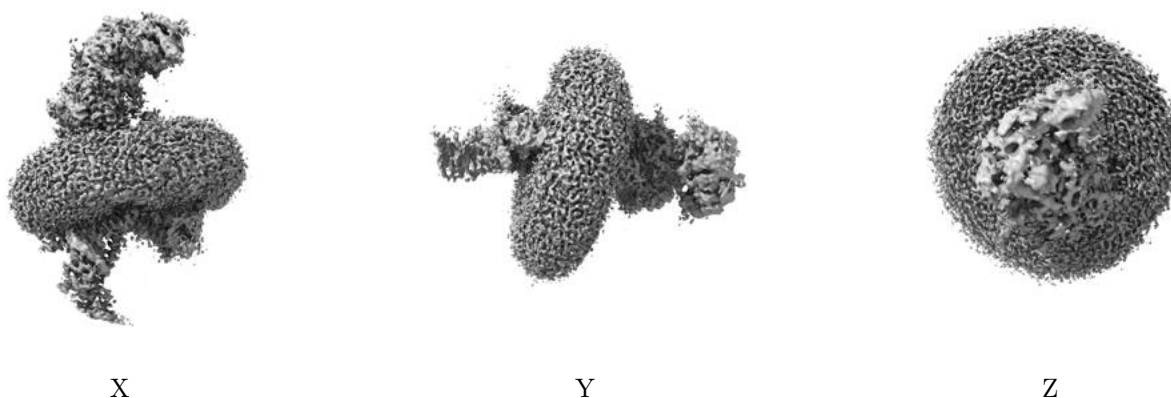


Z

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

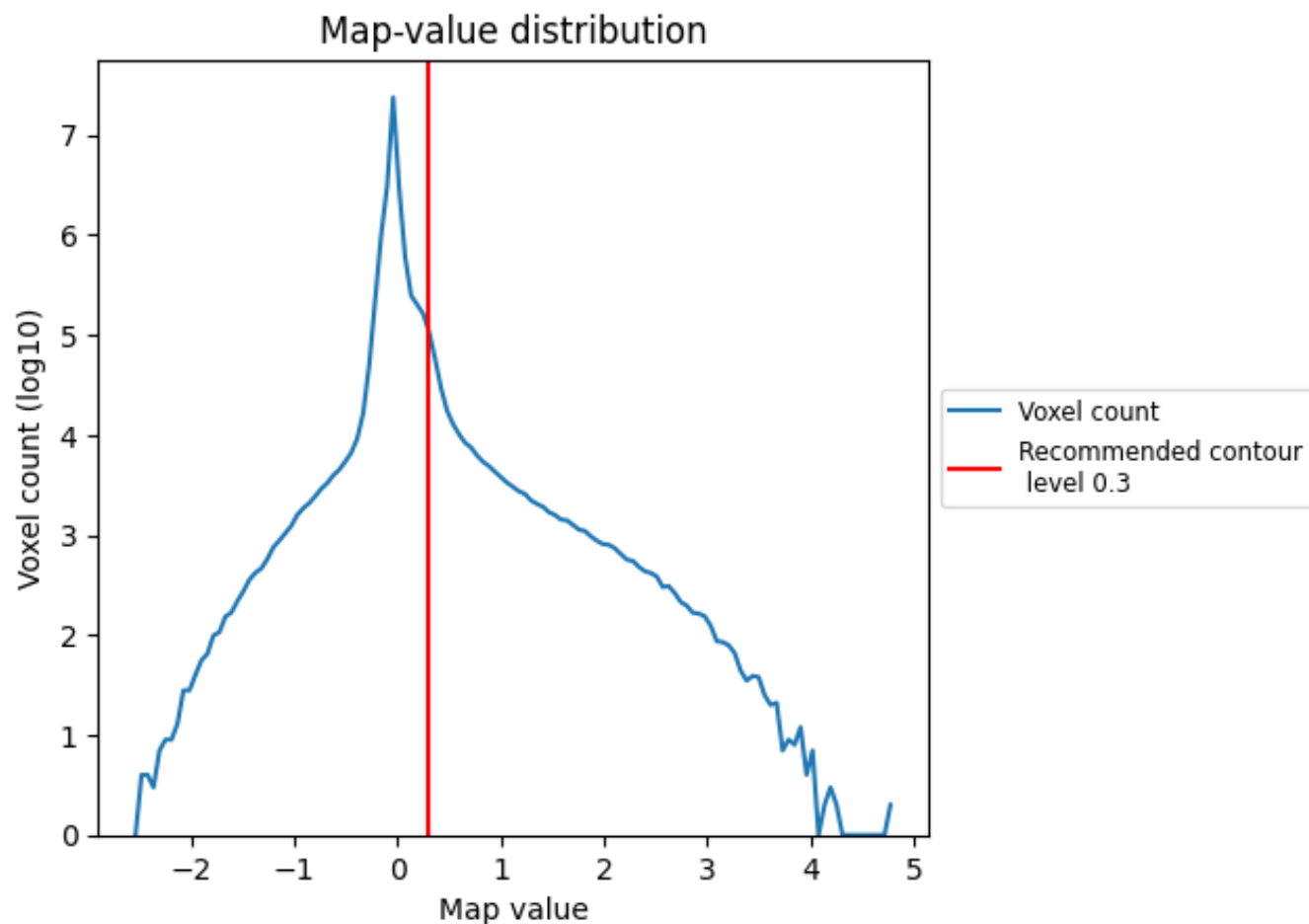
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

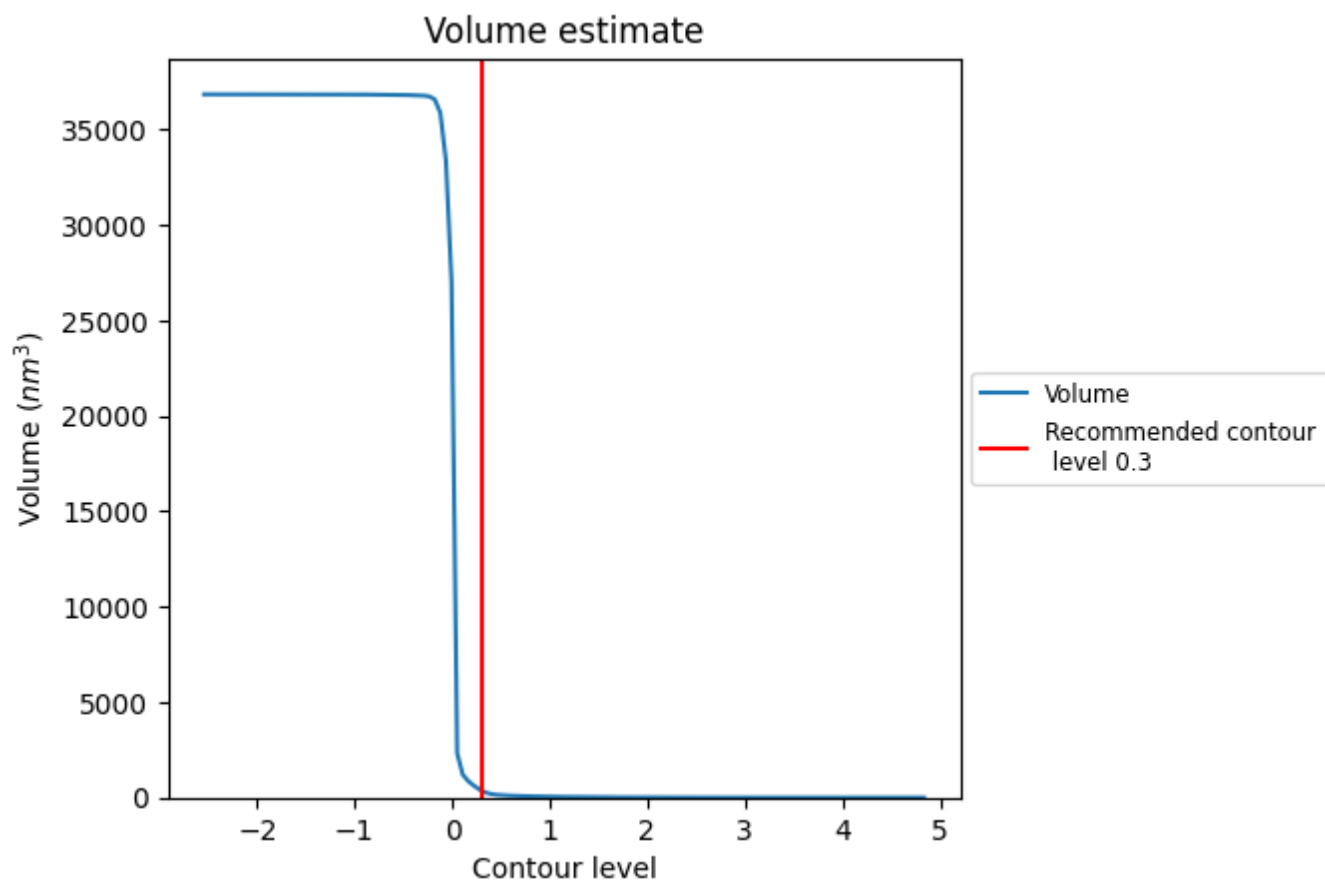
This section contains the results of statistical analysis of the map.

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.

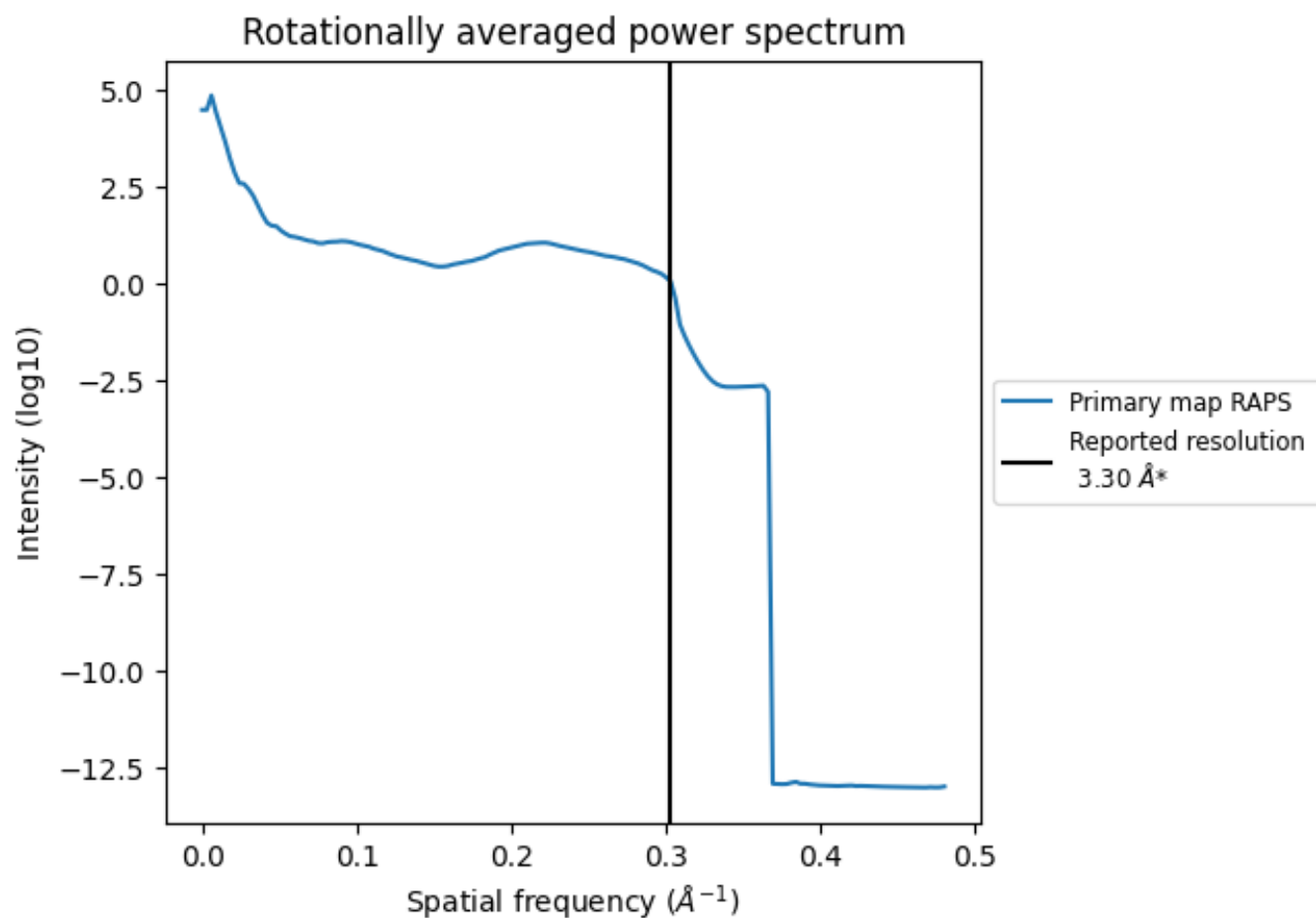
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm^3 ; this corresponds to an approximate mass of 336 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

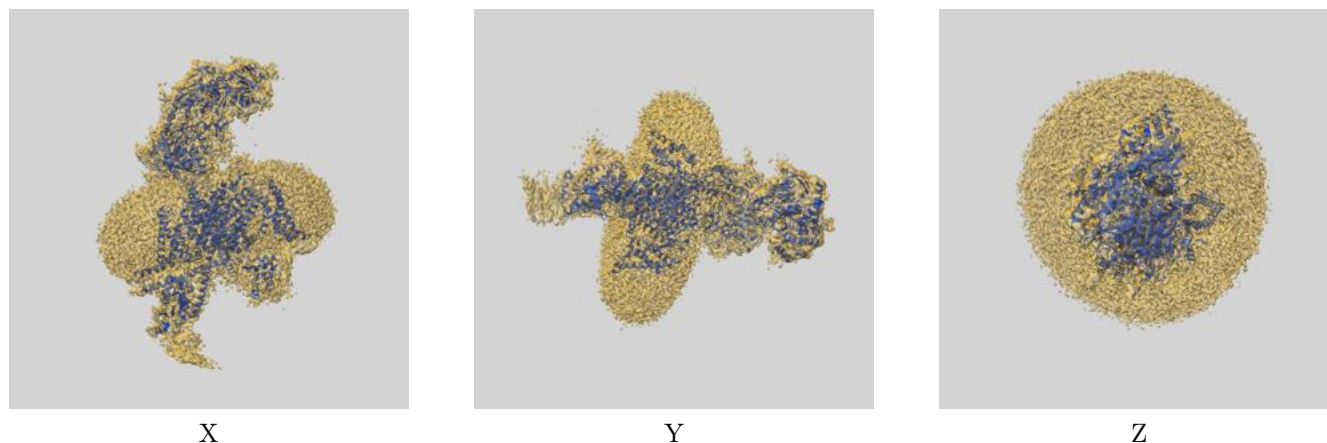
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

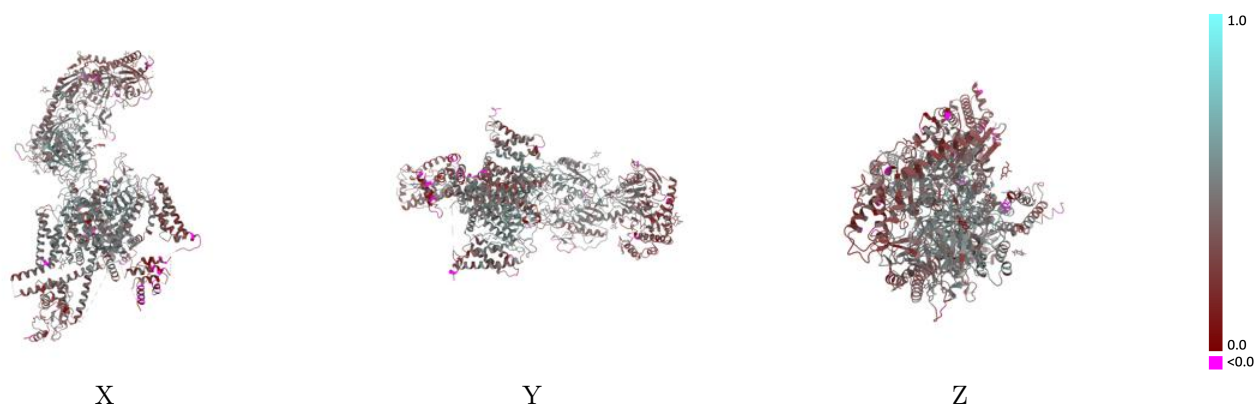
This section contains information regarding the fit between EMDB map EMD-31961 and PDB model 7VFW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 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](#)

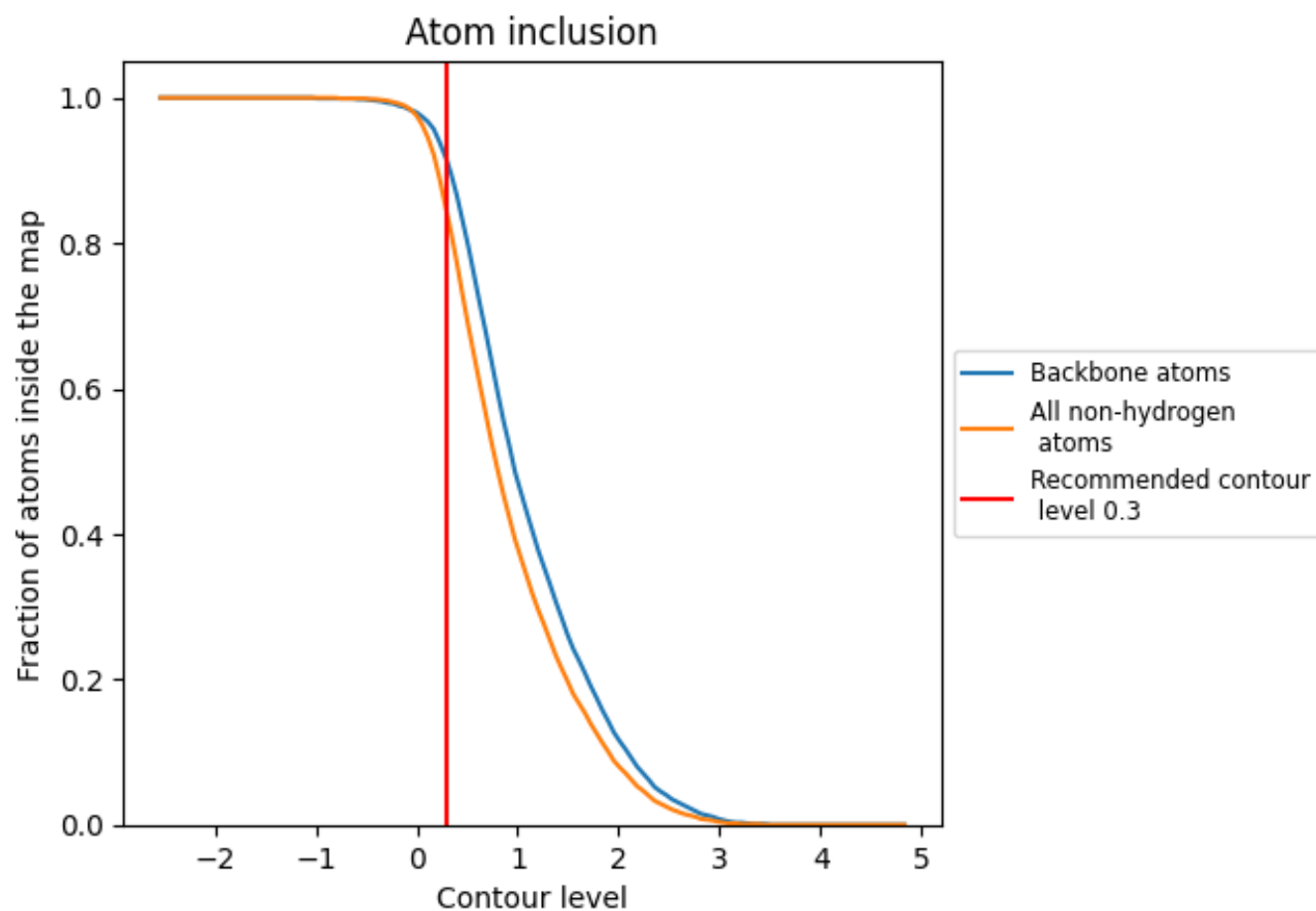


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8410	0.4070
A	0.8570	0.4290
B	0.8370	0.3890
C	0.6670	0.2760
D	0.7330	0.3350
E	0.9230	0.4400
F	0.7440	0.2810

1.0

0.0

<0.0