



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 8WE7 / pdb_00008we7
EMDB ID : EMD-37473
Title : Human L-type voltage-gated calcium channel Cav1.2 in the presence of cal-
ciseptine at 3.2 Angstrom resolution
Authors : Gao, S.; Yao, X.; Yan, N.
Deposited on : 2023-09-17
Resolution : 3.20 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:

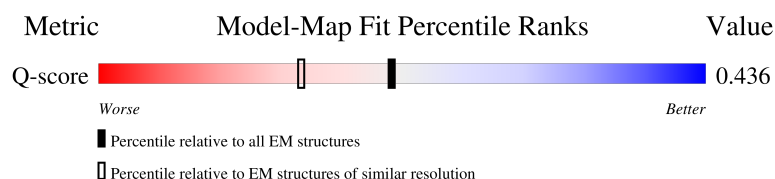
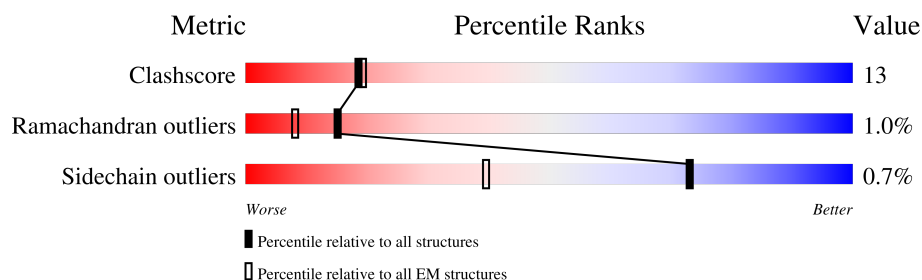
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	2201	15% 40% 17% 43%
2	D	1103	67% 19% 14%
3	C	484	62% 34% 30% 33%
4	B	60	82% 72% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	3	33%100%
6	F	2	50%100%
6	H	2	50%100%
6	I	2	100%
7	G	4	25%75%25%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Voltage-dependent L-type calcium channel subunit alpha-1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1251	Total	C	N	O	S	0	0
			10101	6645	1646	1747	63		

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

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

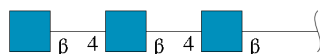
- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

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

- Molecule 4 is a protein called Calciseptin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	60	Total	C	N	O	S	0	0
			486	299	90	87	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			42	24	3	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

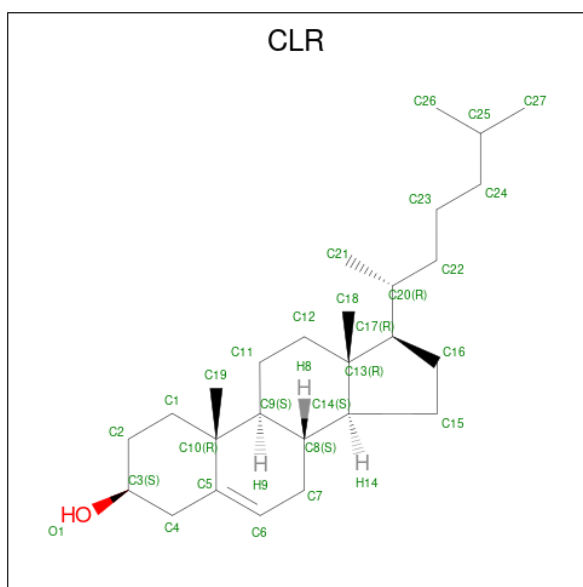


Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

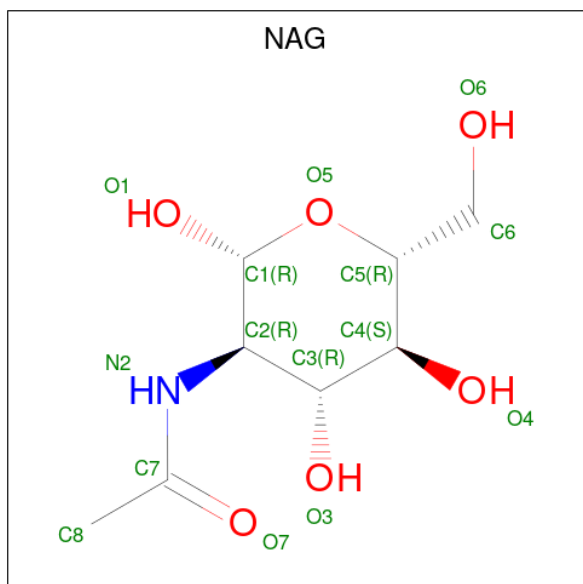
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Ca	0
			1	1	
8	D	1	Total	Ca	0
			1	1	

- Molecule 9 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

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



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

Continued on next page...

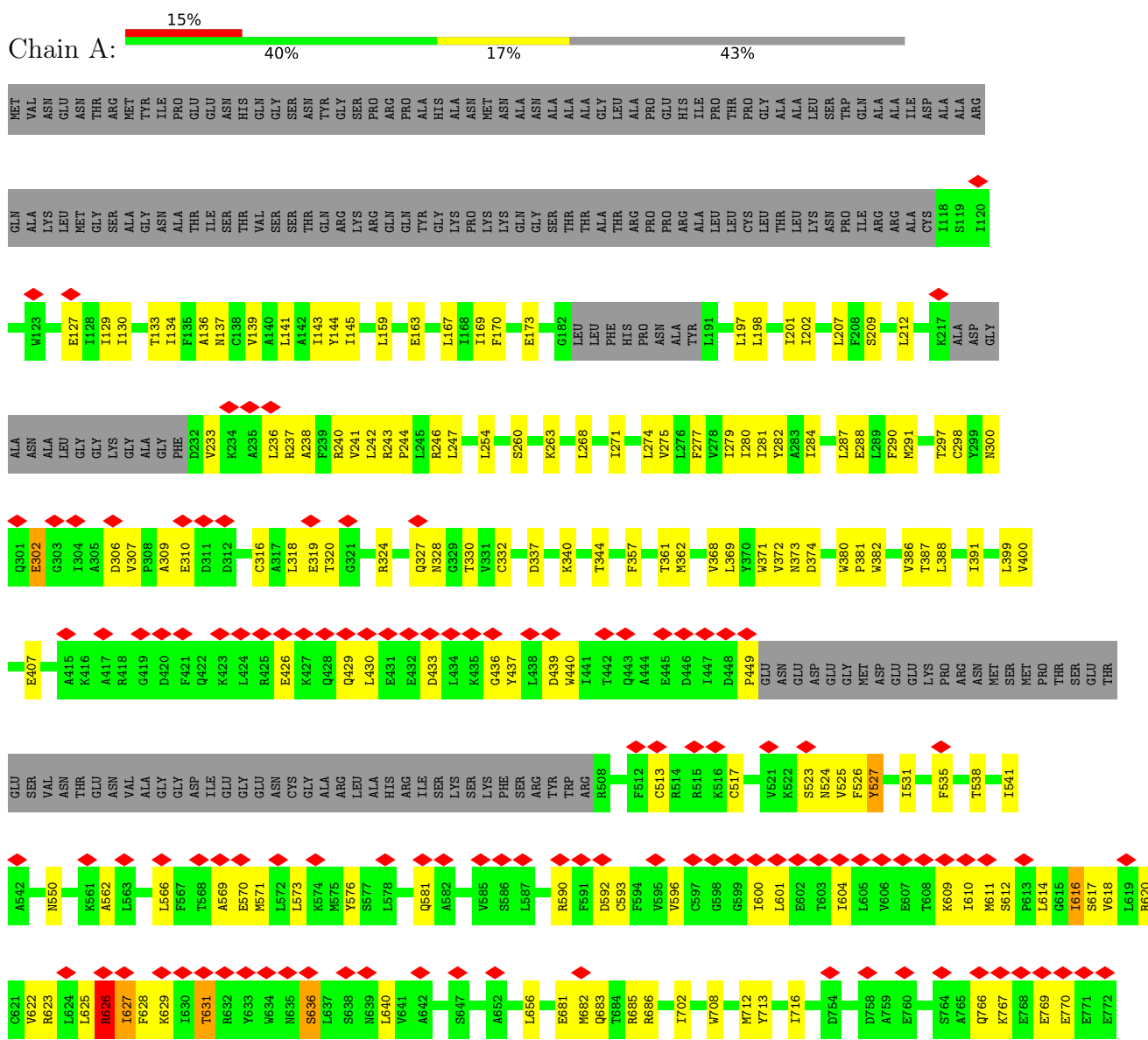
Continued from previous page...

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

3 Residue-property plots

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

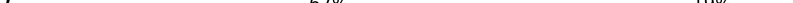
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1C

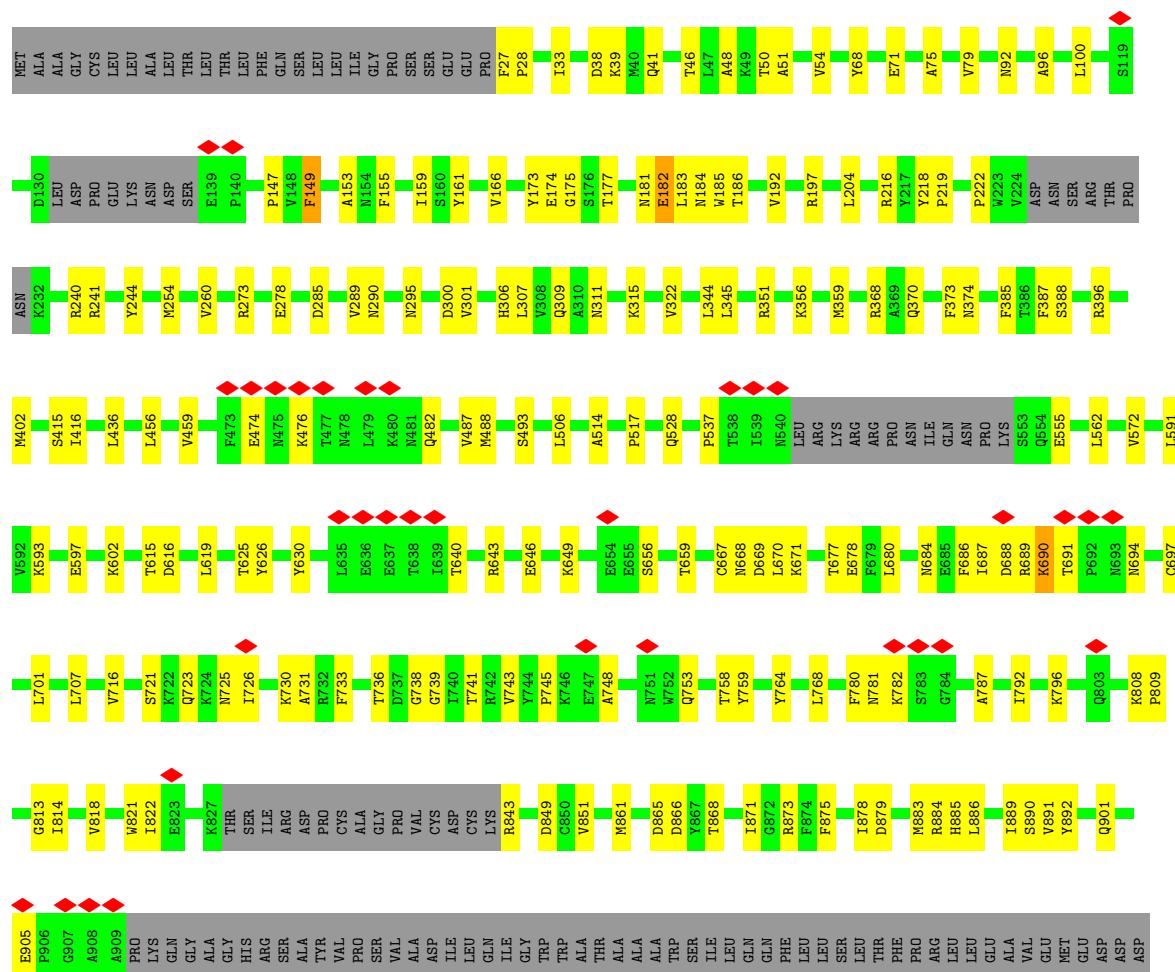


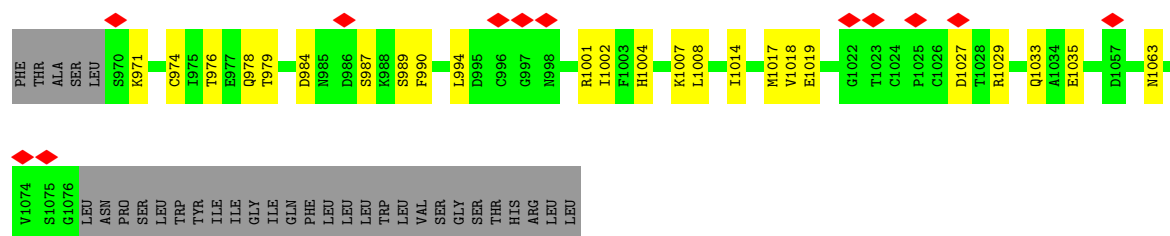


ASP	ARG	GLY	PHE	HIS	ASN	LEU	PRO
ALA	GLY	PHE	PRO	GLN	ARG	LEU	GLY
GLY	ALA	ILE	ILE	ALA	THR	LYS	TYR
GLU	GLN	HIS	HIS	VAL	LEU	ALA	SER
GLU	ASP	CYS	CYS	VAL	PRO	ASN	VAL
ASP	ASP	PRO	GLY	ALA	GLU	THR	GLY
ALA	LYS	PHE	GLY	ALA	SER	SER	THR
GLY	GLY	TRP	TRP	LEU	ASP	ARG	VAL
CYS	CYS	ILE	ALA	SER	LYS	CYS	VAL
VAL	VAL	GLU	GLU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

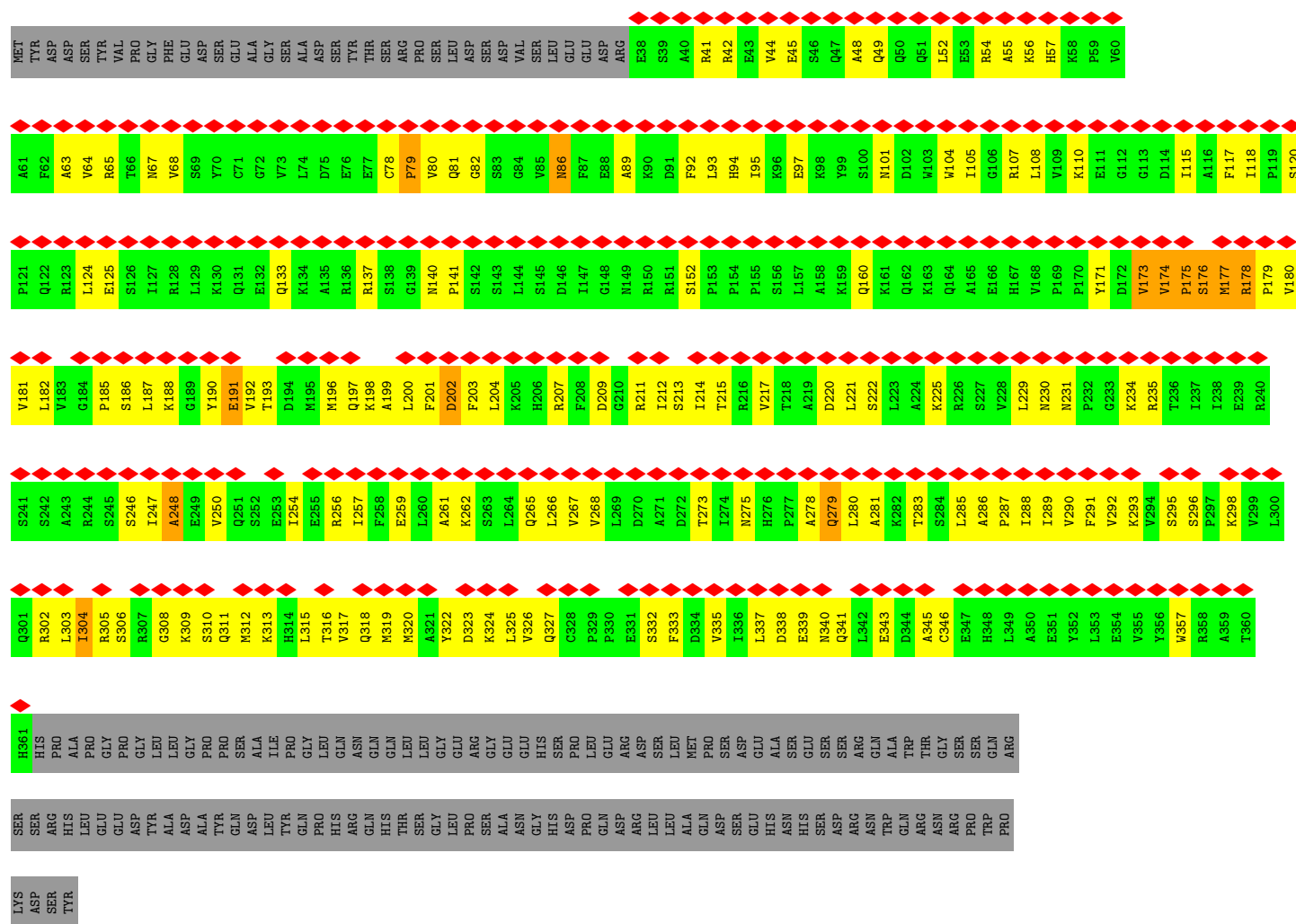
- Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1

Chain D:  67% 19% 14%

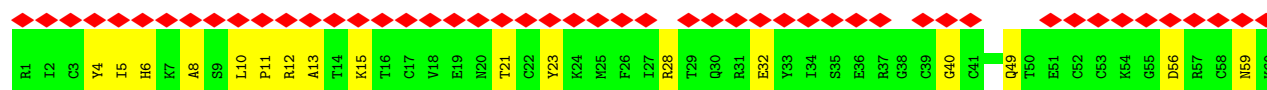
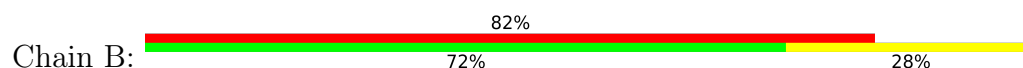




• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3



• Molecule 4: Calciseptin



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

Chain E:  33% 100%



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

Chain F:  50% 100%



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

Chain H:  50% 100%



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

Chain I:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  25% 75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.014	Depositor
Minimum map value	-2.922	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	1/10331 (0.0%)	0.47	6/13997 (0.0%)
2	D	0.16	0/7728	0.36	0/10477
3	C	0.21	0/2624	0.55	3/3544 (0.1%)
4	B	0.12	0/496	0.32	0/664
All	All	0.19	1/21179 (0.0%)	0.44	9/28682 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	TYR	CA-C	-6.54	1.44	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	178	ARG	CA-C-N	-7.34	112.22	119.78
3	C	178	ARG	C-N-CA	-7.34	112.22	119.78
1	A	904	ASN	N-CA-C	-6.63	103.31	111.40
1	A	636	SER	N-CA-C	-6.52	107.19	114.62
1	A	527	TYR	CB-CA-C	-6.52	100.92	110.96
1	A	626	ARG	N-CA-C	-5.94	104.88	111.36
1	A	616	ILE	N-CA-C	-5.70	107.26	112.96
3	C	176	SER	N-CA-C	5.61	118.39	109.24
1	A	1011	ILE	N-CA-C	-5.46	108.52	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10101	0	10330	251	0
2	D	7570	0	7370	146	0
3	C	2575	0	2619	138	0
4	B	486	0	474	13	0
5	E	42	0	37	3	0
6	F	28	0	25	0	0
6	H	28	0	25	0	0
6	I	28	0	25	0	0
7	G	56	0	49	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	A	56	0	92	6	0
10	A	14	0	13	0	0
10	D	28	0	26	1	0
All	All	21014	0	21085	546	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 13.

All (546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:ARG:HB3	3:C:288:ILE:HD11	1.54	0.87
2:D:689:ARG:HG2	2:D:690:LYS:H	1.40	0.86
3:C:316:THR:HA	3:C:319:MET:HE2	1.60	0.82
1:A:1204:LYS:HG3	1:A:1207:ARG:HH21	1.47	0.80
1:A:1310:ILE:HD12	1:A:1379:PHE:HB3	1.63	0.79
1:A:626:ARG:HA	1:A:629:LYS:HD3	1.64	0.79
3:C:304:ILE:HG23	3:C:311:GLN:HE21	1.50	0.76
1:A:1012:ASN:O	1:A:1014:VAL:N	2.20	0.74
3:C:95:ILE:HD13	3:C:105:ILE:H	1.51	0.74
3:C:292:VAL:HG22	3:C:337:LEU:HD22	1.69	0.73
3:C:234:LYS:HG3	3:C:235:ARG:HG2	1.70	0.73
2:D:884:ARG:NH1	2:D:1029:ARG:O	2.22	0.73
2:D:388:SER:OG	2:D:396:ARG:NH1	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:ALA:O	3:C:57:HIS:N	2.22	0.72
1:A:1440:GLU:HG3	1:A:1468:ASP:HB3	1.72	0.72
3:C:125:GLU:O	3:C:160:GLN:NE2	2.23	0.72
3:C:337:LEU:HG	3:C:345:ALA:HB1	1.71	0.71
2:D:240:ARG:NH2	2:D:278:GLU:O	2.23	0.71
4:B:23:TYR:O	4:B:59:ASN:ND2	2.24	0.70
1:A:628:PHE:CE1	1:A:631:THR:HG21	2.27	0.70
2:D:177:THR:O	2:D:181:ASN:ND2	2.24	0.70
3:C:63:ALA:HA	3:C:94:HIS:HA	1.73	0.69
3:C:94:HIS:HB2	3:C:107:ARG:HB3	1.74	0.69
3:C:291:PHE:HB2	3:C:333:PHE:HB3	1.73	0.69
3:C:175:PRO:HB3	3:C:262:LYS:NZ	2.09	0.67
3:C:65:ARG:HG3	3:C:92:PHE:HA	1.75	0.67
3:C:64:VAL:HG22	3:C:171:TYR:CD2	2.30	0.67
1:A:626:ARG:O	1:A:629:LYS:HB2	1.94	0.67
2:D:680:LEU:O	2:D:684:ASN:ND2	2.28	0.67
3:C:214:ILE:HG23	3:C:268:VAL:HB	1.77	0.66
3:C:201:PHE:O	3:C:204:LEU:N	2.24	0.66
1:A:906:ILE:O	1:A:908:PHE:N	2.28	0.66
2:D:689:ARG:HD3	2:D:689:ARG:H	1.61	0.66
3:C:177:MET:HB3	3:C:357:TRP:CH2	2.30	0.66
3:C:182:LEU:HD12	3:C:200:LEU:HD12	1.78	0.66
3:C:178:ARG:HB3	3:C:288:ILE:CD1	2.25	0.65
3:C:312:MET:HA	3:C:315:LEU:HD11	1.78	0.65
3:C:68:VAL:HB	3:C:124:LEU:HD21	1.78	0.64
3:C:247:ILE:HG22	3:C:248:ALA:H	1.62	0.64
2:D:667:CYS:HB3	2:D:697:CYS:HA	1.80	0.64
2:D:528:GLN:O	2:D:901:GLN:NE2	2.31	0.63
2:D:731:ALA:HA	2:D:745:PRO:HG2	1.79	0.63
1:A:426:GLU:HA	1:A:429:GLN:HE21	1.63	0.63
1:A:611:MET:HB3	1:A:614:LEU:HD13	1.79	0.63
3:C:78:CYS:HB3	3:C:117:PHE:HB3	1.80	0.63
2:D:204:LEU:HD13	2:D:456:LEU:HD21	1.79	0.63
3:C:78:CYS:HB2	3:C:82:GLY:HA3	1.81	0.63
1:A:1232:VAL:HG11	1:A:1291:ILE:HG23	1.80	0.63
1:A:1599:ASN:ND2	1:A:1646:MET:SD	2.71	0.63
1:A:281:ILE:HG23	1:A:1381:VAL:HB	1.79	0.63
3:C:179:PRO:HB3	3:C:267:VAL:H	1.63	0.63
2:D:886:LEU:HD22	2:D:891:VAL:HG21	1.80	0.62
1:A:1569:LEU:HD11	1:A:1591:LEU:HD13	1.82	0.62
3:C:78:CYS:O	3:C:80:VAL:N	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1007:LYS:HG2	2:D:1014:ILE:HG22	1.82	0.62
1:A:436:GLY:H	3:C:340:ASN:HD21	1.48	0.61
1:A:1018:ARG:HG3	1:A:1021:ARG:HH12	1.65	0.61
3:C:295:SER:OG	3:C:296:SER:N	2.33	0.61
1:A:1245:MET:HE3	1:A:1285:GLU:HG2	1.83	0.61
1:A:1111:TRP:O	4:B:49:GLN:NE2	2.33	0.61
1:A:1085:THR:HB	1:A:1088:GLU:HG2	1.81	0.61
1:A:913:SER:OG	1:A:1024:ARG:NH1	2.34	0.60
1:A:430:LEU:HD11	3:C:298:LYS:HB2	1.82	0.60
3:C:186:SER:O	3:C:275:ASN:ND2	2.29	0.60
3:C:211:ARG:HB3	3:C:357:TRP:CD1	2.37	0.60
2:D:351:ARG:HH22	2:D:356:LYS:HD3	1.64	0.60
1:A:906:ILE:O	1:A:909:PHE:N	2.35	0.60
2:D:873:ARG:HH11	2:D:878:ILE:HG23	1.65	0.60
1:A:1206:GLN:OE1	1:A:1619:ARG:NH2	2.35	0.60
3:C:278:ALA:O	3:C:280:LEU:N	2.34	0.60
3:C:323:ASP:HA	3:C:327:GLN:HG2	1.83	0.60
1:A:197:LEU:O	1:A:201:ILE:HG13	2.03	0.59
3:C:191:GLU:OE2	3:C:313:LYS:NZ	2.36	0.59
2:D:671:LYS:HA	2:D:671:LYS:HE3	1.85	0.59
1:A:1546:LYS:HG2	1:A:1606:PHE:HZ	1.68	0.59
1:A:1572:ILE:HD12	1:A:1577:GLY:HA3	1.85	0.58
3:C:94:HIS:H	3:C:107:ARG:H	1.51	0.58
3:C:229:LEU:HD12	3:C:231:ASN:H	1.67	0.58
3:C:281:ALA:HA	3:C:287:PRO:HG3	1.86	0.58
1:A:1206:GLN:HE21	1:A:1618:LEU:HD21	1.68	0.58
2:D:260:VAL:HG23	2:D:295:ASN:HB3	1.86	0.58
1:A:426:GLU:OE2	1:A:429:GLN:NE2	2.37	0.57
1:A:906:ILE:C	1:A:908:PHE:N	2.63	0.57
2:D:28:PRO:HG2	2:D:33:ILE:HD11	1.86	0.57
3:C:180:VAL:HG22	3:C:266:LEU:HD22	1.85	0.57
1:A:622:VAL:HA	1:A:625:LEU:HD23	1.85	0.57
1:A:571:MET:HE3	1:A:593:CYS:HA	1.86	0.57
1:A:1249:ILE:O	1:A:1253:THR:HG23	2.04	0.57
2:D:843:ARG:NH1	2:D:865:ASP:OD1	2.37	0.57
3:C:196:MET:SD	3:C:200:LEU:HD21	2.45	0.57
2:D:669:ASP:HB2	2:D:686:PHE:CZ	2.39	0.57
1:A:968:ILE:HD13	1:A:994:LEU:HD23	1.87	0.57
3:C:133:GLN:HG3	3:C:137:ARG:HH11	1.70	0.57
1:A:1220:ARG:NH1	1:A:1554:PRO:O	2.37	0.56
2:D:68:TYR:HB3	2:D:707:LEU:HD21	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:LEU:HD13	3:C:292:VAL:HG21	1.87	0.56
1:A:1137:TRP:CD1	1:A:1138:PRO:HD3	2.41	0.56
1:A:1202:LEU:HG	1:A:1207:ARG:HG2	1.87	0.56
1:A:902:PHE:HA	1:A:905:LEU:HD22	1.88	0.56
1:A:297:THR:O	1:A:332:CYS:HB2	2.05	0.56
1:A:996:VAL:HG12	1:A:1023:LEU:HB2	1.87	0.56
1:A:523:SER:O	1:A:525:VAL:N	2.37	0.56
1:A:380:TRP:N	1:A:381:PRO:HD3	2.20	0.56
2:D:891:VAL:HG22	2:D:990:PHE:CD2	2.40	0.56
1:A:167:LEU:HD21	1:A:207:LEU:HD13	1.87	0.55
3:C:212:ILE:HG23	3:C:266:LEU:HG	1.87	0.55
1:A:337:ASP:N	1:A:337:ASP:OD1	2.38	0.55
2:D:100:LEU:HB2	2:D:488:MET:HE2	1.88	0.55
1:A:130:ILE:O	1:A:134:ILE:HG13	2.07	0.55
3:C:266:LEU:HD23	3:C:357:TRP:CZ3	2.41	0.55
1:A:238:ALA:O	1:A:241:VAL:HG22	2.07	0.55
1:A:1232:VAL:HG12	1:A:1292:ALA:HB2	1.88	0.55
1:A:1177:MET:HE3	1:A:1177:MET:HA	1.89	0.55
2:D:161:TYR:CE2	2:D:197:ARG:HD2	2.41	0.55
2:D:684:ASN:HA	2:D:687:ILE:HG22	1.88	0.55
1:A:1382:MET:O	1:A:1385:VAL:HG12	2.08	0.55
3:C:65:ARG:HH12	3:C:178:ARG:HD3	1.71	0.55
2:D:506:LEU:O	2:D:759:TYR:OH	2.22	0.54
1:A:449:PRO:HA	3:C:198:LYS:HE3	1.87	0.54
1:A:1417:MET:O	1:A:1421:ILE:HG12	2.07	0.54
1:A:1376:PHE:HA	1:A:1379:PHE:CE2	2.42	0.54
3:C:201:PHE:O	3:C:203:PHE:N	2.41	0.54
1:A:254:LEU:HD11	1:A:656:LEU:HD23	1.88	0.54
1:A:906:ILE:O	1:A:907:LEU:C	2.50	0.54
2:D:688:ASP:N	2:D:688:ASP:OD1	2.41	0.54
1:A:531:ILE:HD11	1:A:626:ARG:HB2	1.89	0.54
3:C:290:VAL:HG12	3:C:335:VAL:HB	1.88	0.54
1:A:902:PHE:HA	1:A:905:LEU:HB2	1.89	0.54
2:D:517:PRO:HG3	2:D:616:ASP:HB2	1.90	0.54
2:D:359:MET:HE3	2:D:385:PHE:HB2	1.89	0.54
1:A:380:TRP:O	1:A:380:TRP:HE3	1.91	0.53
1:A:1135:GLU:HB3	1:A:1467:GLN:HE22	1.72	0.53
1:A:1185:VAL:HG12	1:A:1520:VAL:HG11	1.90	0.53
1:A:1275:ASN:O	1:A:1279:THR:HG23	2.08	0.53
1:A:1459:ARG:HE	1:A:1469:ILE:HD11	1.73	0.53
2:D:615:THR:OG1	2:D:616:ASP:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:PHE:CE1	1:A:1382:MET:HB3	2.44	0.53
2:D:885:HIS:O	2:D:889:ILE:HG22	2.08	0.53
3:C:199:ALA:HA	3:C:202:ASP:HB2	1.91	0.53
3:C:192:VAL:O	3:C:196:MET:HB3	2.09	0.53
1:A:1592:VAL:HA	1:A:1596:MET:HE1	1.90	0.53
2:D:736:THR:HG23	2:D:738:GLY:H	1.73	0.53
3:C:177:MET:O	3:C:178:ARG:C	2.52	0.53
3:C:217:VAL:HG11	3:C:256:ARG:HH12	1.72	0.53
1:A:1233:TRP:HA	1:A:1292:ALA:HB1	1.90	0.53
2:D:27:PHE:N	2:D:28:PRO:HD3	2.24	0.53
2:D:753:GLN:OE1	2:D:753:GLN:N	2.42	0.53
3:C:305:ARG:HB3	3:C:311:GLN:HE22	1.74	0.53
2:D:182:GLU:O	2:D:184:ASN:N	2.42	0.53
3:C:65:ARG:HD3	3:C:174:VAL:HG23	1.91	0.52
1:A:1029:ILE:HG23	1:A:1035:LEU:HG	1.91	0.52
1:A:1269:ILE:O	1:A:1273:ILE:HG12	2.09	0.52
3:C:229:LEU:CD1	3:C:231:ASN:H	2.23	0.52
1:A:439:ASP:OD1	1:A:440:TRP:N	2.42	0.52
2:D:301:VAL:HG23	2:D:301:VAL:O	2.09	0.52
3:C:215:THR:HG23	3:C:267:VAL:HG13	1.91	0.52
2:D:723:GLN:NE2	2:D:725:ASN:O	2.38	0.52
1:A:1644:THR:HB	1:A:1647:LYS:HB3	1.92	0.52
3:C:187:LEU:HD21	3:C:317:VAL:HG22	1.92	0.52
1:A:318:LEU:O	1:A:320:THR:N	2.42	0.52
1:A:274:LEU:HD13	1:A:1398:LEU:HD21	1.91	0.52
1:A:284:ILE:O	1:A:288:GLU:HG2	2.10	0.52
2:D:48:ALA:HA	2:D:814:ILE:HD12	1.90	0.52
2:D:290:ASN:ND2	2:D:306:HIS:O	2.43	0.52
1:A:373:ASN:OD1	1:A:381:PRO:HG2	2.10	0.52
1:A:1063:PHE:HA	1:A:1066:ILE:HD12	1.92	0.51
3:C:65:ARG:CZ	3:C:92:PHE:HB3	2.39	0.51
3:C:67:ASN:HA	3:C:89:ALA:HA	1.91	0.51
1:A:324:ARG:HB2	1:A:374:ASP:HB2	1.92	0.51
2:D:92:ASN:OD1	10:D:1202:NAG:N2	2.42	0.51
1:A:1546:LYS:HG2	1:A:1606:PHE:CZ	2.45	0.51
2:D:51:ALA:HB2	2:D:726:ILE:HG21	1.91	0.51
1:A:531:ILE:HG21	1:A:627:ILE:HG12	1.91	0.51
2:D:990:PHE:O	2:D:1004:HIS:ND1	2.40	0.51
1:A:778:LEU:O	1:A:782:ALA:N	2.35	0.51
3:C:289:ILE:HD13	3:C:332:SER:HB2	1.91	0.51
1:A:198:LEU:HA	1:A:201:ILE:HD12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:LEU:HD22	1:A:1514:LEU:HD12	1.91	0.51
2:D:54:VAL:HG21	2:D:796:LYS:HG3	1.93	0.51
2:D:285:ASP:O	2:D:309:GLN:NE2	2.39	0.51
2:D:311:ASN:O	2:D:315:LYS:HB2	2.10	0.51
2:D:818:VAL:O	2:D:822:ILE:HG13	2.11	0.51
1:A:1231:LYS:O	1:A:1235:VAL:HG23	2.11	0.51
3:C:175:PRO:HB3	3:C:262:LYS:HZ2	1.75	0.51
1:A:340:LYS:HD2	1:A:371:TRP:HH2	1.76	0.50
1:A:686:ARG:HE	1:A:1142:TYR:HB3	1.76	0.50
1:A:998:SER:HA	1:A:1001:LEU:HB2	1.93	0.50
2:D:562:LEU:HD11	2:D:572:VAL:HG22	1.92	0.50
3:C:178:ARG:HD2	3:C:286:ALA:HB3	1.93	0.50
2:D:373:PHE:HE2	2:D:402:MET:HG2	1.75	0.50
1:A:139:VAL:O	1:A:143:ILE:HD12	2.12	0.50
1:A:901:ILE:HG22	1:A:905:LEU:HD22	1.93	0.50
1:A:1029:ILE:HA	1:A:1035:LEU:HD23	1.92	0.50
1:A:437:TYR:N	3:C:340:ASN:OD1	2.44	0.50
1:A:1224:PRO:HG2	1:A:1230:TYR:HA	1.92	0.50
2:D:51:ALA:HB3	2:D:814:ILE:HD11	1.94	0.50
2:D:979:THR:O	2:D:1033:GLN:NE2	2.32	0.50
3:C:178:ARG:HH11	3:C:286:ALA:C	2.20	0.50
1:A:277:PHE:HD1	1:A:1388:LEU:HB2	1.76	0.50
1:A:541:ILE:HD12	1:A:617:SER:HB2	1.93	0.50
1:A:1221:ARG:HG3	1:A:1551:GLU:HA	1.94	0.50
1:A:1310:ILE:CD1	1:A:1379:PHE:HB3	2.37	0.50
2:D:886:LEU:O	2:D:891:VAL:HB	2.11	0.50
1:A:129:ILE:O	1:A:133:THR:HG23	2.11	0.50
1:A:569:ALA:O	1:A:573:LEU:HG	2.12	0.50
1:A:1212:TYR:OH	1:A:1543:ASP:OD1	2.29	0.50
2:D:153:ALA:O	2:D:155:PHE:N	2.45	0.50
2:D:537:PRO:HD3	2:D:974:CYS:HB3	1.93	0.50
2:D:640:THR:HG22	2:D:643:ARG:HH12	1.76	0.50
4:B:5:ILE:HB	4:B:15:LYS:HB3	1.94	0.50
1:A:912:LEU:O	1:A:915:ILE:HG12	2.10	0.50
1:A:1316:ILE:HA	1:A:1319:ILE:HB	1.93	0.50
3:C:65:ARG:HG2	3:C:92:PHE:HD1	1.76	0.50
1:A:407:GLU:OE2	1:A:407:GLU:HA	2.13	0.49
1:A:1023:LEU:HA	1:A:1026:LEU:HD12	1.93	0.49
1:A:1090:LYS:HB3	2:D:173:TYR:CD2	2.48	0.49
1:A:1283:THR:O	1:A:1287:ILE:HG12	2.11	0.49
2:D:173:TYR:HD1	2:D:175:GLY:H	1.58	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PHE:HE2	1:A:243:ARG:HD3	1.78	0.49
1:A:767:LYS:HA	1:A:770:GLU:HG3	1.93	0.49
3:C:180:VAL:HG12	3:C:288:ILE:HB	1.94	0.49
4:B:6:HIS:NE2	4:B:12:ARG:HA	2.27	0.49
1:A:260:SER:HA	1:A:263:LYS:HD2	1.94	0.49
1:A:1040:GLN:O	1:A:1044:VAL:HG23	2.12	0.49
2:D:459:VAL:HG12	2:D:493:SER:HA	1.93	0.49
2:D:46:THR:O	2:D:50:THR:HG22	2.12	0.49
1:A:1033:LYS:HA	1:A:1036:LYS:HE2	1.94	0.48
1:A:1202:LEU:HD21	1:A:1637:ILE:HD11	1.95	0.48
2:D:978:GLN:NE2	2:D:1035:GLU:OE2	2.30	0.48
4:B:6:HIS:ND1	4:B:8:ALA:O	2.41	0.48
1:A:627:ILE:HD13	1:A:627:ILE:HA	1.63	0.48
2:D:646:GLU:HA	2:D:649:LYS:HG2	1.95	0.48
3:C:215:THR:HG21	3:C:257:ILE:HD11	1.95	0.48
1:A:280:ILE:HG22	1:A:1384:LEU:HD21	1.96	0.48
3:C:52:LEU:HB3	3:C:115:ILE:HG21	1.96	0.48
2:D:733:PHE:HB3	2:D:743:VAL:HG22	1.96	0.48
3:C:316:THR:O	3:C:319:MET:HG2	2.14	0.48
1:A:1424:VAL:HA	1:A:1427:MET:HE2	1.94	0.48
2:D:344:LEU:O	2:D:345:LEU:HD23	2.13	0.48
3:C:222:SER:HG	3:C:273:THR:HG1	1.55	0.48
3:C:254:ILE:HD13	3:C:285:LEU:HD21	1.95	0.48
1:A:198:LEU:O	1:A:202:ILE:HG23	2.13	0.48
1:A:904:ASN:O	1:A:906:ILE:N	2.47	0.48
2:D:976:THR:OG1	2:D:1035:GLU:OE1	2.27	0.48
3:C:193:THR:O	3:C:197:GLN:N	2.36	0.48
3:C:322:TYR:O	3:C:326:VAL:HG12	2.14	0.48
1:A:1541:HIS:O	1:A:1544:GLU:HG3	2.13	0.48
2:D:307:LEU:HD12	2:D:351:ARG:HH11	1.78	0.48
2:D:668:ASN:OD1	2:D:668:ASN:N	2.47	0.47
2:D:764:TYR:OH	2:D:809:PRO:O	2.31	0.47
1:A:368:VAL:O	1:A:372:VAL:HG23	2.13	0.47
1:A:1006:ILE:O	1:A:1007:GLN:HG2	2.13	0.47
1:A:1148:HIS:NE2	1:A:1153:GLY:O	2.48	0.47
1:A:1228:HIS:O	1:A:1232:VAL:HG23	2.14	0.47
3:C:108:LEU:HG	3:C:110:LYS:HG2	1.97	0.47
3:C:175:PRO:HB3	3:C:262:LYS:HZ3	1.80	0.47
3:C:225:LYS:HA	3:C:283:THR:HA	1.95	0.47
2:D:677:THR:OG1	2:D:678:GLU:OE1	2.33	0.47
1:A:241:VAL:C	1:A:244:PRO:HD2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:OH	1:A:626:ARG:HB3	2.15	0.47
1:A:906:ILE:HD11	1:A:967:GLU:HG3	1.95	0.47
2:D:149:PHE:CZ	2:D:222:PRO:HD3	2.50	0.47
2:D:415:SER:OG	2:D:416:ILE:N	2.47	0.47
3:C:52:LEU:HD11	3:C:117:PHE:CE2	2.50	0.47
1:A:137:ASN:O	1:A:141:LEU:HG	2.14	0.47
1:A:382:TRP:O	1:A:386:VAL:HG12	2.15	0.47
2:D:591:LEU:HD23	2:D:602:LYS:HG2	1.97	0.47
2:D:891:VAL:HG22	2:D:990:PHE:HD2	1.80	0.47
1:A:297:THR:C	1:A:332:CYS:HB2	2.40	0.47
2:D:555:GLU:OE2	2:D:555:GLU:N	2.47	0.47
3:C:185:PRO:HD3	3:C:291:PHE:HE1	1.80	0.47
2:D:745:PRO:HB2	2:D:748:ALA:HB3	1.96	0.47
3:C:304:ILE:HD11	3:C:318:GLN:HE21	1.80	0.47
2:D:730:LYS:HB2	2:D:730:LYS:HE2	1.60	0.46
3:C:256:ARG:O	3:C:259:GLU:HG2	2.16	0.46
1:A:344:THR:OG1	1:A:713:TYR:OH	2.29	0.46
1:A:681:GLU:OE1	1:A:685:ARG:NH2	2.48	0.46
1:A:243:ARG:HB3	1:A:244:PRO:HD3	1.97	0.46
1:A:1191:GLU:O	1:A:1195:GLN:HB2	2.15	0.46
3:C:63:ALA:O	3:C:173:VAL:HA	2.15	0.46
1:A:300:ASN:O	1:A:302:GLU:HG3	2.14	0.46
1:A:1474:MET:HE1	1:A:1501:VAL:HG23	1.97	0.46
2:D:669:ASP:HB2	2:D:686:PHE:HZ	1.79	0.46
1:A:1640:ILE:HG13	1:A:1642:LYS:H	1.81	0.46
2:D:273:ARG:HG2	2:D:322:VAL:O	2.16	0.46
2:D:890:SER:OG	2:D:984:ASP:OD1	2.32	0.46
3:C:310:SER:C	3:C:312:MET:H	2.24	0.46
1:A:1216:ALA:HB1	1:A:1606:PHE:HE2	1.80	0.46
3:C:320:MET:O	3:C:324:LYS:N	2.42	0.46
2:D:359:MET:HE2	2:D:387:PHE:HE1	1.79	0.46
2:D:373:PHE:CE2	2:D:402:MET:HG2	2.50	0.46
2:D:689:ARG:HG2	2:D:690:LYS:N	2.20	0.46
4:B:56:ASP:N	4:B:56:ASP:OD1	2.49	0.46
1:A:592:ASP:HB2	1:A:623:ARG:HD3	1.97	0.46
1:A:1200:CYS:O	1:A:1201:GLU:HG2	2.16	0.46
3:C:64:VAL:N	3:C:93:LEU:O	2.43	0.46
3:C:220:ASP:H	3:C:250:VAL:HG12	1.81	0.46
1:A:779:ALA:O	1:A:783:SER:OG	2.27	0.46
1:A:1378:LEU:O	1:A:1381:VAL:HG22	2.16	0.46
2:D:174:GLU:OE2	2:D:174:GLU:N	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:HA	3:C:97:GLU:HG3	1.98	0.45
3:C:283:THR:HG23	3:C:285:LEU:H	1.81	0.45
2:D:597:GLU:HG2	2:D:978:GLN:HE22	1.80	0.45
4:B:10:LEU:HB2	4:B:11:PRO:HD3	1.97	0.45
2:D:733:PHE:CZ	2:D:813:GLY:HA3	2.51	0.45
1:A:369:LEU:O	1:A:373:ASN:HB2	2.16	0.45
1:A:144:TYR:HA	1:A:159:LEU:HD12	1.98	0.45
2:D:33:ILE:HG13	2:D:1017:MET:HE1	1.98	0.45
2:D:989:SER:C	2:D:990:PHE:HD1	2.25	0.45
3:C:64:VAL:O	3:C:64:VAL:HG13	2.16	0.45
1:A:1068:VAL:O	1:A:1072:LYS:HB2	2.17	0.45
1:A:300:ASN:H	1:A:330:THR:HG23	1.80	0.45
1:A:437:TYR:CD2	3:C:303:LEU:HD12	2.52	0.45
3:C:44:VAL:O	3:C:48:ALA:N	2.38	0.45
3:C:217:VAL:HG11	3:C:256:ARG:NH1	2.32	0.45
5:E:2:NAG:H4	5:E:3:NAG:H2	1.43	0.45
1:A:1433:ILE:HA	1:A:1479:CYS:HA	1.98	0.45
1:A:297:THR:CA	1:A:316:CYS:SG	3.05	0.45
1:A:1049:ILE:HG12	1:A:1181:PHE:CD1	2.52	0.45
1:A:275:VAL:O	1:A:279:ILE:HG13	2.17	0.45
3:C:104:TRP:O	3:C:118:ILE:N	2.49	0.45
3:C:305:ARG:HB2	3:C:308:GLY:O	2.17	0.45
3:C:337:LEU:O	3:C:337:LEU:HD23	2.17	0.45
1:A:136:ALA:O	1:A:139:VAL:HG12	2.17	0.44
1:A:298:CYS:HB3	1:A:330:THR:HG22	1.99	0.44
1:A:307:VAL:O	1:A:307:VAL:HG13	2.16	0.44
3:C:181:VAL:N	3:C:288:ILE:O	2.48	0.44
3:C:209:ASP:HA	3:C:212:ILE:O	2.17	0.44
4:B:21:THR:O	4:B:40:GLY:N	2.49	0.44
9:A:2302:CLR:H9	9:A:2303:CLR:H111	1.99	0.44
2:D:244:TYR:CD1	2:D:487:VAL:HB	2.52	0.44
2:D:368:ARG:HB3	2:D:370:GLN:HG3	1.98	0.44
2:D:868:THR:O	2:D:871:ILE:HG13	2.18	0.44
1:A:233:VAL:O	1:A:237:ARG:HG3	2.17	0.44
1:A:1018:ARG:HG3	1:A:1021:ARG:NH1	2.31	0.44
3:C:124:LEU:HB2	3:C:171:TYR:HE1	1.81	0.44
3:C:133:GLN:HG3	3:C:137:ARG:NH1	2.32	0.44
4:B:59:ASN:OD1	4:B:59:ASN:N	2.50	0.44
1:A:1022:VAL:HG11	1:A:1425:ILE:HG13	2.00	0.44
2:D:182:GLU:C	2:D:184:ASN:N	2.75	0.44
1:A:1036:LYS:HB2	1:A:1036:LYS:HE3	1.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:TYR:HB3	1:A:1100:GLU:O	2.17	0.44
1:A:1250:LEU:HD23	1:A:1250:LEU:HA	1.79	0.44
1:A:1537:LEU:HD12	1:A:1537:LEU:HA	1.85	0.44
1:A:576:TYR:HD1	1:A:576:TYR:H	1.66	0.44
1:A:968:ILE:O	1:A:972:MET:N	2.48	0.44
2:D:701:LEU:HD23	2:D:701:LEU:HA	1.87	0.44
2:D:987:SER:HB2	2:D:990:PHE:HE1	1.82	0.44
3:C:86:ASN:C	3:C:86:ASN:HD22	2.26	0.44
1:A:1426:GLY:HA2	1:A:1430:PHE:HD1	1.83	0.44
9:A:2303:CLR:H162	9:A:2303:CLR:H221	1.62	0.44
2:D:41:GLN:HB2	2:D:1008:LEU:HD23	2.00	0.44
3:C:48:ALA:O	3:C:52:LEU:HD13	2.17	0.44
4:B:6:HIS:CE1	4:B:12:ARG:HA	2.53	0.44
1:A:173:GLU:OE1	1:A:246:ARG:NH2	2.50	0.44
1:A:904:ASN:C	1:A:906:ILE:N	2.73	0.44
1:A:1054:ILE:HD13	1:A:1054:ILE:HA	1.87	0.44
2:D:849:ASP:N	2:D:1018:VAL:O	2.50	0.44
3:C:101:ASN:O	3:C:120:SER:OG	2.25	0.44
3:C:246:SER:O	3:C:247:ILE:HD13	2.18	0.44
1:A:357:PHE:O	1:A:361:THR:HG23	2.18	0.44
2:D:290:ASN:HB2	2:D:307:LEU:HD23	2.00	0.44
2:D:716:VAL:O	2:D:721:SER:HB3	2.18	0.44
3:C:65:ARG:HD3	3:C:174:VAL:CG2	2.47	0.44
3:C:124:LEU:HD22	3:C:171:TYR:CE1	2.53	0.44
1:A:1093:TYR:HB3	1:A:1109:ARG:HH11	1.83	0.43
1:A:1312:ILE:HA	1:A:1315:ILE:HD12	2.00	0.43
2:D:723:GLN:HG2	2:D:726:ILE:HD13	2.00	0.43
2:D:994:LEU:HD22	2:D:1001:ARG:HD3	2.00	0.43
1:A:1376:PHE:HA	1:A:1379:PHE:HE2	1.81	0.43
1:A:1403:LYS:HG3	1:A:1404:SER:N	2.33	0.43
2:D:781:ASN:O	2:D:782:LYS:HG3	2.18	0.43
3:C:63:ALA:HB1	3:C:65:ARG:HE	1.84	0.43
1:A:914:SER:O	1:A:917:LEU:HG	2.18	0.43
1:A:975:TYR:HD2	1:A:986:ARG:HH21	1.66	0.43
1:A:1306:PHE:HE1	1:A:1382:MET:HB3	1.83	0.43
1:A:1316:ILE:HD11	1:A:1376:PHE:CE2	2.53	0.43
2:D:241:ARG:HA	2:D:241:ARG:HD2	1.86	0.43
3:C:221:LEU:H	3:C:273:THR:HG21	1.83	0.43
1:A:133:THR:HG21	1:A:169:ILE:HG21	2.00	0.43
1:A:1212:TYR:HE1	1:A:1546:LYS:HE2	1.82	0.43
2:D:1002:ILE:HG13	2:D:1019:GLU:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1027:ASP:OD1	2:D:1027:ASP:N	2.52	0.43
3:C:254:ILE:HA	3:C:257:ILE:HG22	2.00	0.43
3:C:305:ARG:O	3:C:305:ARG:HG2	2.18	0.43
1:A:298:CYS:HB2	1:A:309:ALA:HB2	2.01	0.43
2:D:474:GLU:HG3	2:D:476:LYS:HG2	2.01	0.43
3:C:80:VAL:O	3:C:81:GLN:HB3	2.19	0.43
1:A:562:ALA:O	1:A:566:LEU:HD23	2.19	0.43
1:A:702:ILE:HG23	1:A:708:TRP:HB2	2.00	0.43
1:A:1511:CYS:O	1:A:1515:ILE:HG12	2.18	0.43
3:C:41:ARG:HG2	3:C:42:ARG:N	2.33	0.43
1:A:324:ARG:CB	1:A:374:ASP:HB2	2.47	0.43
1:A:614:LEU:HG	1:A:616:ILE:HG23	1.99	0.43
1:A:1113:ASN:OD1	1:A:1114:SER:N	2.51	0.43
1:A:1524:MET:SD	1:A:1524:MET:N	2.91	0.43
2:D:821:TRP:CG	2:D:861:MET:HE2	2.53	0.43
2:D:851:VAL:HG21	2:D:875:PHE:CZ	2.53	0.43
3:C:190:TYR:O	3:C:193:THR:N	2.47	0.43
3:C:302:ARG:O	3:C:305:ARG:NH1	2.51	0.43
1:A:209:SER:HA	1:A:236:LEU:HD13	2.01	0.43
1:A:922:PRO:HG3	1:A:1427:MET:CG	2.49	0.43
2:D:166:VAL:HG11	2:D:183:LEU:HD21	2.00	0.43
2:D:182:GLU:O	2:D:183:LEU:C	2.59	0.43
1:A:387:THR:O	1:A:391:ILE:HB	2.19	0.43
1:A:766:GLN:O	1:A:769:GLU:HG3	2.19	0.43
2:D:821:TRP:CD2	2:D:861:MET:HE2	2.54	0.43
3:C:343:GLU:O	3:C:346:CYS:HB2	2.18	0.43
1:A:271:ILE:HD13	1:A:399:LEU:HB3	2.00	0.43
1:A:636:SER:O	1:A:640:LEU:N	2.50	0.43
1:A:712:MET:O	1:A:716:ILE:HG13	2.19	0.43
1:A:1002:ILE:O	1:A:1006:ILE:HG13	2.19	0.43
1:A:1549:TRP:HZ2	1:A:1560:ILE:HG21	1.84	0.43
2:D:300:ASP:N	2:D:300:ASP:OD1	2.52	0.43
2:D:875:PHE:O	2:D:883:MET:HB2	2.19	0.43
3:C:179:PRO:HA	3:C:266:LEU:HB2	2.00	0.43
1:A:1246:PHE:HZ	1:A:1390:ARG:HE	1.67	0.42
1:A:1634:ARG:HD3	1:A:1640:ILE:HG12	2.01	0.42
2:D:75:ALA:O	2:D:79:VAL:HG23	2.19	0.42
2:D:100:LEU:HD23	2:D:192:VAL:HB	2.01	0.42
2:D:796:LYS:HD2	2:D:796:LYS:HA	1.71	0.42
3:C:105:ILE:HG23	3:C:115:ILE:HG23	2.01	0.42
4:B:4:TYR:HB2	4:B:13:ALA:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:OD1	1:A:550:ASN:C	2.62	0.42
1:A:1159:ARG:HD2	1:A:1162:ILE:HB	2.01	0.42
2:D:436:LEU:HD21	2:D:482:GLN:HG2	2.01	0.42
3:C:78:CYS:HA	3:C:79:PRO:HD2	1.76	0.42
1:A:268:LEU:HD21	1:A:400:VAL:HA	2.01	0.42
1:A:163:GLU:OE1	1:A:240:ARG:NH1	2.53	0.42
1:A:433:ASP:HA	3:C:340:ASN:CG	2.44	0.42
1:A:618:VAL:O	1:A:620:ARG:N	2.51	0.42
1:A:922:PRO:HG3	1:A:1427:MET:SD	2.59	0.42
2:D:818:VAL:HG22	2:D:822:ILE:HD11	2.00	0.42
4:B:28:ARG:H	4:B:28:ARG:HG2	1.61	0.42
1:A:1245:MET:HA	1:A:1245:MET:HE2	2.00	0.42
1:A:1310:ILE:HD13	1:A:1310:ILE:HA	1.93	0.42
1:A:1453:ALA:O	1:A:1457:LEU:HG	2.19	0.42
1:A:1587:ALA:O	1:A:1590:ARG:HG3	2.19	0.42
2:D:625:THR:OG1	2:D:626:TYR:N	2.51	0.42
2:D:686:PHE:CD1	2:D:690:LYS:HG2	2.55	0.42
2:D:781:ASN:CG	2:D:782:LYS:N	2.78	0.42
1:A:277:PHE:HB3	1:A:1388:LEU:HD22	2.00	0.42
1:A:297:THR:HA	1:A:316:CYS:SG	2.60	0.42
1:A:1280:GLY:O	1:A:1283:THR:OG1	2.32	0.42
2:D:514:ALA:HB2	2:D:619:LEU:HD12	2.01	0.42
3:C:188:LYS:HD3	3:C:188:LYS:HA	1.75	0.42
1:A:590:ARG:HA	1:A:593:CYS:HB3	2.02	0.42
1:A:686:ARG:NH2	1:A:1146:ASP:OD1	2.53	0.42
1:A:989:PHE:CG	1:A:1030:ASN:HB2	2.54	0.42
2:D:593:LYS:HD2	2:D:597:GLU:HG3	2.02	0.42
2:D:780:PHE:CD1	2:D:781:ASN:N	2.77	0.42
1:A:1250:LEU:O	1:A:1254:ILE:HG13	2.20	0.42
1:A:1428:GLN:OE1	1:A:1428:GLN:HA	2.19	0.42
1:A:1557:LYS:HB3	1:A:1558:GLY:H	1.70	0.42
1:A:1581:LEU:HD13	1:A:1585:ARG:HH12	1.84	0.42
3:C:309:LYS:HB3	3:C:310:SER:H	1.72	0.42
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.87	0.42
1:A:513:CYS:O	1:A:517:CYS:HB2	2.19	0.42
1:A:1526:ASN:HD21	1:A:1529:TYR:HD2	1.67	0.42
2:D:182:GLU:HA	2:D:185:TRP:CD1	2.55	0.42
2:D:656:SER:HA	2:D:716:VAL:HG11	2.02	0.42
3:C:176:SER:HB2	3:C:261:ALA:O	2.20	0.42
3:C:247:ILE:HG22	3:C:248:ALA:N	2.31	0.42
1:A:596:VAL:O	1:A:600:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:MET:HG3	1:A:683:GLN:N	2.35	0.42
1:A:1225:LYS:HG2	1:A:1226:ASN:H	1.85	0.42
2:D:38:ASP:OD1	2:D:39:LYS:N	2.53	0.42
3:C:141:PRO:HB3	3:C:152:SER:O	2.20	0.42
1:A:134:ILE:HG21	1:A:247:LEU:HB2	2.02	0.41
3:C:293:LYS:HG2	3:C:338:ASP:HB2	2.01	0.41
1:A:535:PHE:HA	1:A:538:THR:HG22	2.02	0.41
1:A:1005:GLY:O	1:A:1007:GLN:N	2.50	0.41
1:A:1208:GLN:O	1:A:1211:GLU:HG2	2.20	0.41
1:A:1392:GLU:H	1:A:1392:GLU:HG2	1.63	0.41
1:A:1457:LEU:HB3	1:A:1507:PHE:CZ	2.55	0.41
3:C:104:TRP:N	3:C:118:ILE:O	2.45	0.41
1:A:242:LEU:HD21	9:A:2303:CLR:H25	2.02	0.41
2:D:436:LEU:HB2	2:D:1063:ASN:ND2	2.36	0.41
2:D:792:ILE:HD13	2:D:821:TRP:HZ3	1.84	0.41
2:D:905:GLU:HA	2:D:971:LYS:HA	2.02	0.41
3:C:213:SER:HB3	3:C:265:GLN:OE1	2.20	0.41
3:C:309:LYS:O	3:C:310:SER:HB3	2.19	0.41
5:E:3:NAG:O7	5:E:3:NAG:O4	2.30	0.41
2:D:159:ILE:CD1	2:D:161:TYR:HE1	2.33	0.41
2:D:659:THR:HA	2:D:741:THR:O	2.21	0.41
1:A:1187:VAL:O	1:A:1191:GLU:HG3	2.21	0.41
1:A:1256:LEU:HD23	1:A:1256:LEU:O	2.21	0.41
2:D:218:TYR:CD1	2:D:219:PRO:HA	2.56	0.41
2:D:739:GLY:HA2	2:D:758:THR:HG23	2.02	0.41
1:A:327:GLN:HB3	1:A:328:ASN:H	1.63	0.41
1:A:601:LEU:O	1:A:604:ILE:HG22	2.20	0.41
1:A:916:SER:HB2	1:A:953:LEU:HD22	2.03	0.41
1:A:1029:ILE:HG12	1:A:1417:MET:HE1	2.02	0.41
3:C:140:ASN:N	3:C:141:PRO:HD2	2.35	0.41
1:A:380:TRP:O	1:A:380:TRP:CE3	2.74	0.41
1:A:1090:LYS:HB3	2:D:173:TYR:CE2	2.56	0.41
2:D:71:GLU:HB2	2:D:630:TYR:CE1	2.55	0.41
2:D:891:VAL:HG22	2:D:990:PHE:CE2	2.55	0.41
3:C:93:LEU:HD23	3:C:118:ILE:HG13	2.02	0.41
1:A:1115:LYS:HG3	1:A:1471:LEU:HD11	2.03	0.41
9:A:2302:CLR:H12	9:A:2303:CLR:H193	2.02	0.41
2:D:690:LYS:O	2:D:691:THR:C	2.64	0.41
1:A:282:TYR:CE2	1:A:388:LEU:HB2	2.55	0.41
1:A:902:PHE:HA	1:A:905:LEU:CD2	2.50	0.41
1:A:1217:ARG:HG3	1:A:1218:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:LYS:HA	1:A:1231:LYS:HD2	1.74	0.41
2:D:186:THR:O	2:D:216:ARG:NH1	2.54	0.41
2:D:254:MET:O	2:D:289:VAL:HA	2.21	0.41
2:D:768:LEU:HD22	2:D:808:LYS:HB3	2.03	0.41
2:D:987:SER:O	2:D:1007:LYS:HD3	2.21	0.41
5:E:2:NAG:H61	5:E:3:NAG:O5	2.20	0.41
2:D:96:ALA:O	2:D:100:LEU:HD12	2.21	0.41
3:C:203:PHE:O	3:C:207:ARG:N	2.51	0.41
3:C:279:GLN:HG3	3:C:280:LEU:H	1.86	0.41
3:C:339:GLU:HG2	3:C:341:GLN:HG2	2.03	0.41
4:B:32:GLU:H	4:B:32:GLU:HG2	1.63	0.41
1:A:992:LEU:O	1:A:996:VAL:HG13	2.20	0.40
1:A:1586:VAL:HA	1:A:1589:LYS:HB2	2.03	0.40
2:D:147:PRO:HG2	2:D:149:PHE:CZ	2.55	0.40
2:D:891:VAL:HG12	2:D:892:TYR:CD1	2.56	0.40
3:C:178:ARG:NH2	3:C:288:ILE:HG13	2.35	0.40
1:A:287:LEU:O	1:A:291:MET:HB2	2.20	0.40
1:A:290:PHE:HE1	1:A:380:TRP:HZ3	1.70	0.40
1:A:526:PHE:HZ	1:A:570:GLU:HG2	1.85	0.40
1:A:1215:LYS:HG3	1:A:1215:LYS:O	2.21	0.40
2:D:359:MET:HE2	2:D:387:PHE:CE1	2.56	0.40
3:C:175:PRO:HB2	3:C:176:SER:H	1.51	0.40
3:C:325:LEU:HD12	3:C:326:VAL:HB	2.01	0.40
1:A:362:MET:HE2	1:A:362:MET:HB2	1.87	0.40
1:A:581:GLN:NE2	3:C:306:SER:O	2.54	0.40
1:A:628:PHE:CD1	1:A:631:THR:HG21	2.55	0.40
1:A:1207:ARG:NH2	1:A:1208:GLN:HE22	2.19	0.40
2:D:878:ILE:HG13	2:D:879:ASP:OD1	2.21	0.40
3:C:320:MET:O	3:C:324:LYS:HG3	2.22	0.40
1:A:1443:ARG:H	1:A:1443:ARG:HG3	1.60	0.40
9:A:2302:CLR:H12	9:A:2303:CLR:H11	2.02	0.40
9:A:2303:CLR:H262	9:A:2303:CLR:H231	1.89	0.40
2:D:873:ARG:NH1	2:D:878:ILE:HG23	2.34	0.40
3:C:45:GLU:O	3:C:49:GLN:N	2.38	0.40
1:A:127:GLU:O	1:A:130:ILE:HG22	2.22	0.40
1:A:429:GLN:H	1:A:429:GLN:HG2	1.63	0.40
1:A:1317:ASP:HA	1:A:1320:LEU:HG	2.03	0.40
1:A:1519:PHE:O	1:A:1523:ILE:HG13	2.20	0.40
2:D:670:LEU:HG	2:D:686:PHE:CD2	2.56	0.40
2:D:987:SER:HB2	2:D:990:PHE:CE1	2.57	0.40
3:C:104:TRP:HA	3:C:104:TRP:CE3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1235/2201 (56%)	1109 (90%)	114 (9%)	12 (1%)	12	45
2	D	936/1103 (85%)	848 (91%)	83 (9%)	5 (0%)	24	59
3	C	322/484 (66%)	261 (81%)	52 (16%)	9 (3%)	4	25
4	B	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
All	All	2551/3848 (66%)	2272 (89%)	253 (10%)	26 (1%)	15	45

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ILE
1	A	302	GLU
2	D	787	ALA
2	D	866	ASP
3	C	56	LYS
3	C	79	PRO
3	C	175	PRO
3	C	191	GLU
3	C	202	ASP
3	C	279	GLN
1	A	310	GLU
1	A	610	ILE
1	A	612	SER
1	A	907	LEU
1	A	1013	VAL
2	D	690	LYS
3	C	177	MET
1	A	524	ASN
1	A	609	LYS
1	A	1227	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	54	ARG
3	C	248	ALA
1	A	319	GLU
1	A	1557	LYS
2	D	149	PHE
2	D	694	ASN

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	1109/1896 (58%)	1099 (99%)	10 (1%)	70	81
2	D	837/971 (86%)	835 (100%)	2 (0%)	87	89
3	C	287/426 (67%)	282 (98%)	5 (2%)	53	75
4	B	54/54 (100%)	54 (100%)	0	100	100
All	All	2287/3347 (68%)	2270 (99%)	17 (1%)	73	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	626	ARG
1	A	627	ILE
1	A	631	THR
1	A	905	LEU
1	A	997	VAL
1	A	1176	PHE
1	A	1281	LEU
1	A	1449	THR
1	A	1628	GLN
2	D	182	GLU
2	D	374	ASN
3	C	86	ASN
3	C	173	VAL
3	C	174	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	230	ASN
3	C	304	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	GLN
1	A	678	ASN
1	A	766	GLN
1	A	924	GLN
1	A	1030	ASN
1	A	1259	GLN
1	A	1445	ASN
1	A	1584	HIS
1	A	1628	GLN
1	A	1630	ASN
2	D	311	ASN
2	D	377	ASN
2	D	424	GLN
2	D	595	GLN
2	D	652	ASN
2	D	718	ASN
2	D	870	GLN
3	C	51	GLN
3	C	86	ASN
3	C	167	HIS
3	C	197	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 ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	E	1	5,2	14,14,15	0.72	0	17,19,21	2.20	3 (17%)
5	NAG	E	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	E	3	5	14,14,15	0.59	0	17,19,21	0.89	0
6	NAG	F	1	6,2	14,14,15	0.45	0	17,19,21	0.57	0
6	NAG	F	2	6	14,14,15	0.49	0	17,19,21	0.78	0
7	NAG	G	1	7,2	14,14,15	0.28	0	17,19,21	0.51	0
7	NAG	G	2	7	14,14,15	0.22	0	17,19,21	0.54	0
7	NAG	G	3	7	14,14,15	1.02	1 (7%)	17,19,21	1.10	1 (5%)
7	NAG	G	4	7	14,14,15	0.32	0	17,19,21	0.35	0
6	NAG	H	1	6,2	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	H	2	6	14,14,15	0.30	0	17,19,21	0.52	0
6	NAG	I	1	6,2	14,14,15	0.49	0	17,19,21	0.39	0
6	NAG	I	2	6	14,14,15	0.22	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	3	5	-	3/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	4/6/23/26	0/1/1/1
7	NAG	G	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	NAG	G	3	7	-	3/6/23/26	0/1/1/1
7	NAG	G	4	7	-	2/6/23/26	0/1/1/1
6	NAG	H	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1
6	NAG	I	1	6,2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	NAG	O5-C1	3.34	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	8.26	123.25	112.19
7	G	3	NAG	C1-O5-C5	4.16	117.76	112.19
5	E	1	NAG	O5-C5-C4	2.50	116.91	110.83
5	E	1	NAG	C3-C4-C5	2.32	114.44	110.23

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	NAG	C1-C2-N2-C7
6	H	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
7	G	3	NAG	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
7	G	3	NAG	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
7	G	4	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
6	I	1	NAG	C8-C7-N2-C2
6	I	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

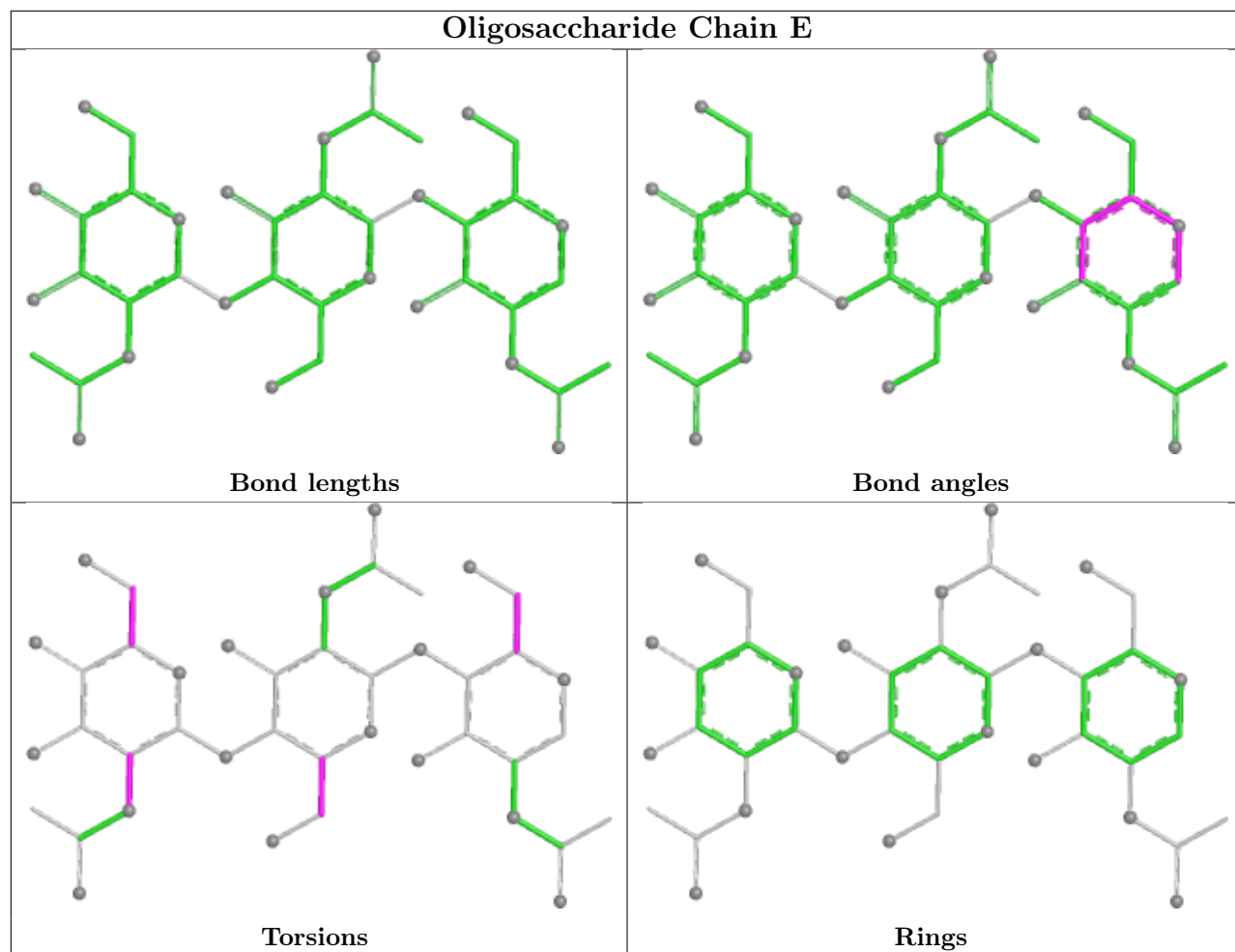
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
5	E	3	NAG	O5-C5-C6-O6
7	G	4	NAG	C4-C5-C6-O6
7	G	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
6	F	2	NAG	C1-C2-N2-C7
7	G	3	NAG	C3-C2-N2-C7
6	F	2	NAG	C3-C2-N2-C7

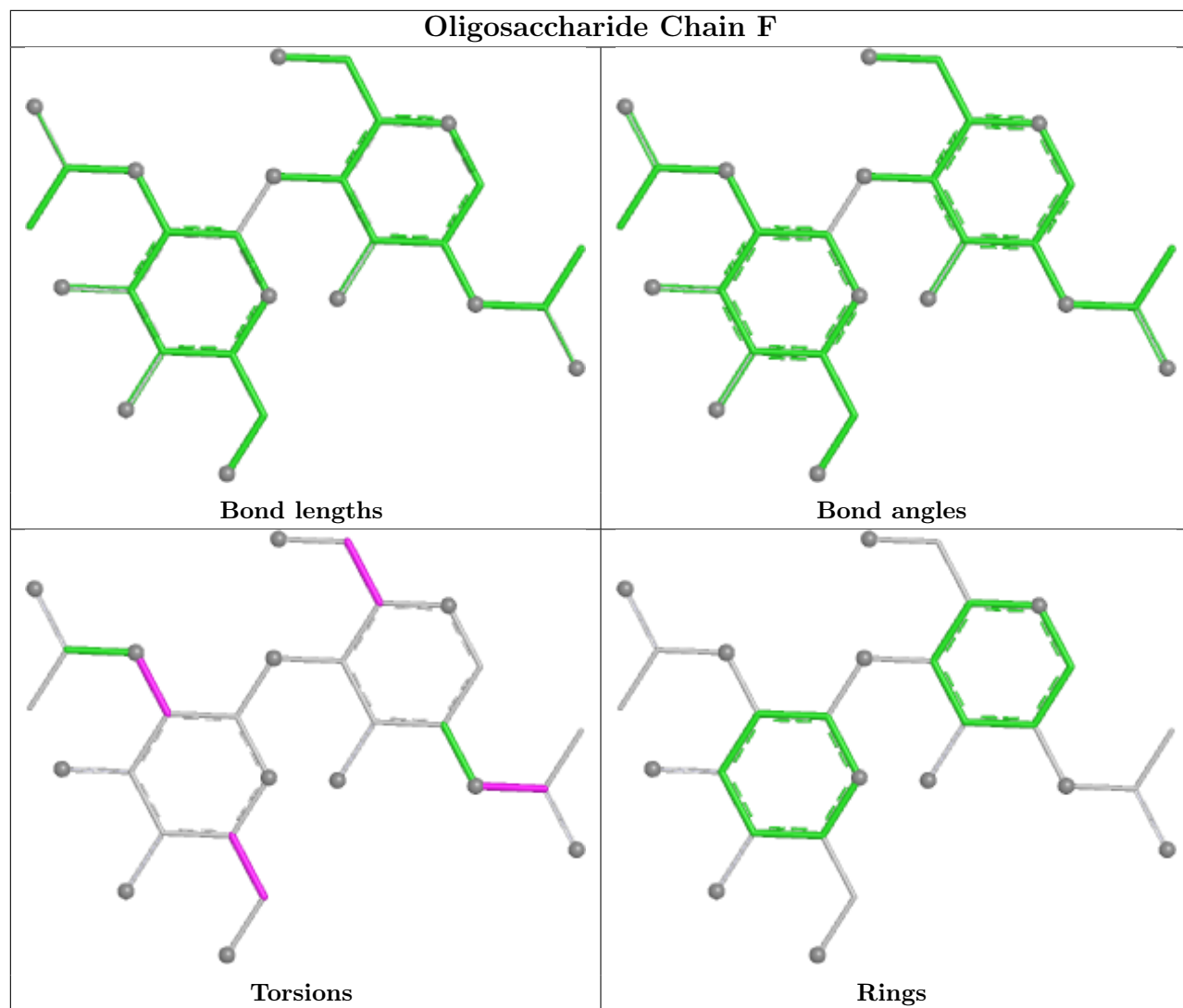
There are no ring outliers.

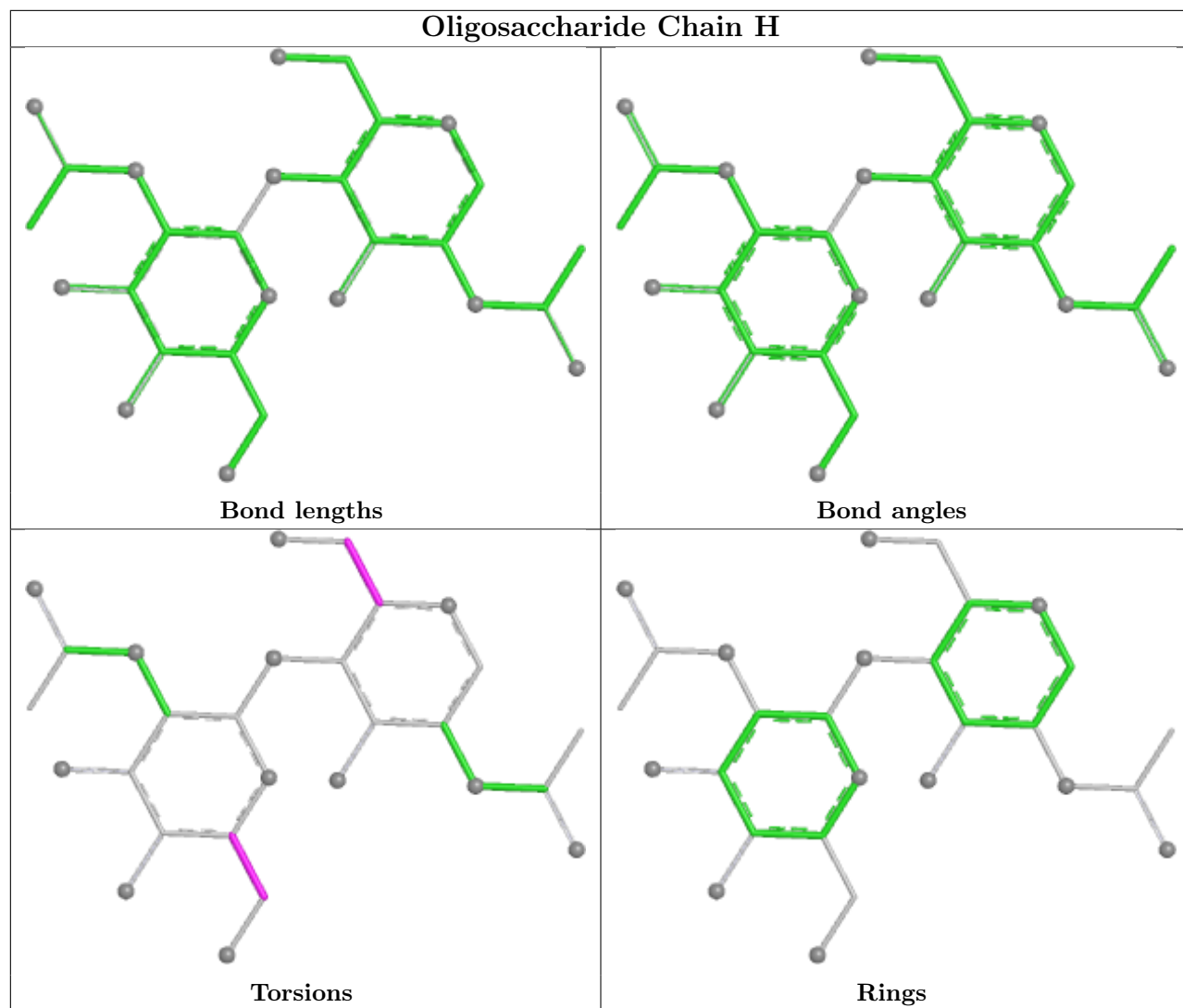
2 monomers are involved in 3 short contacts:

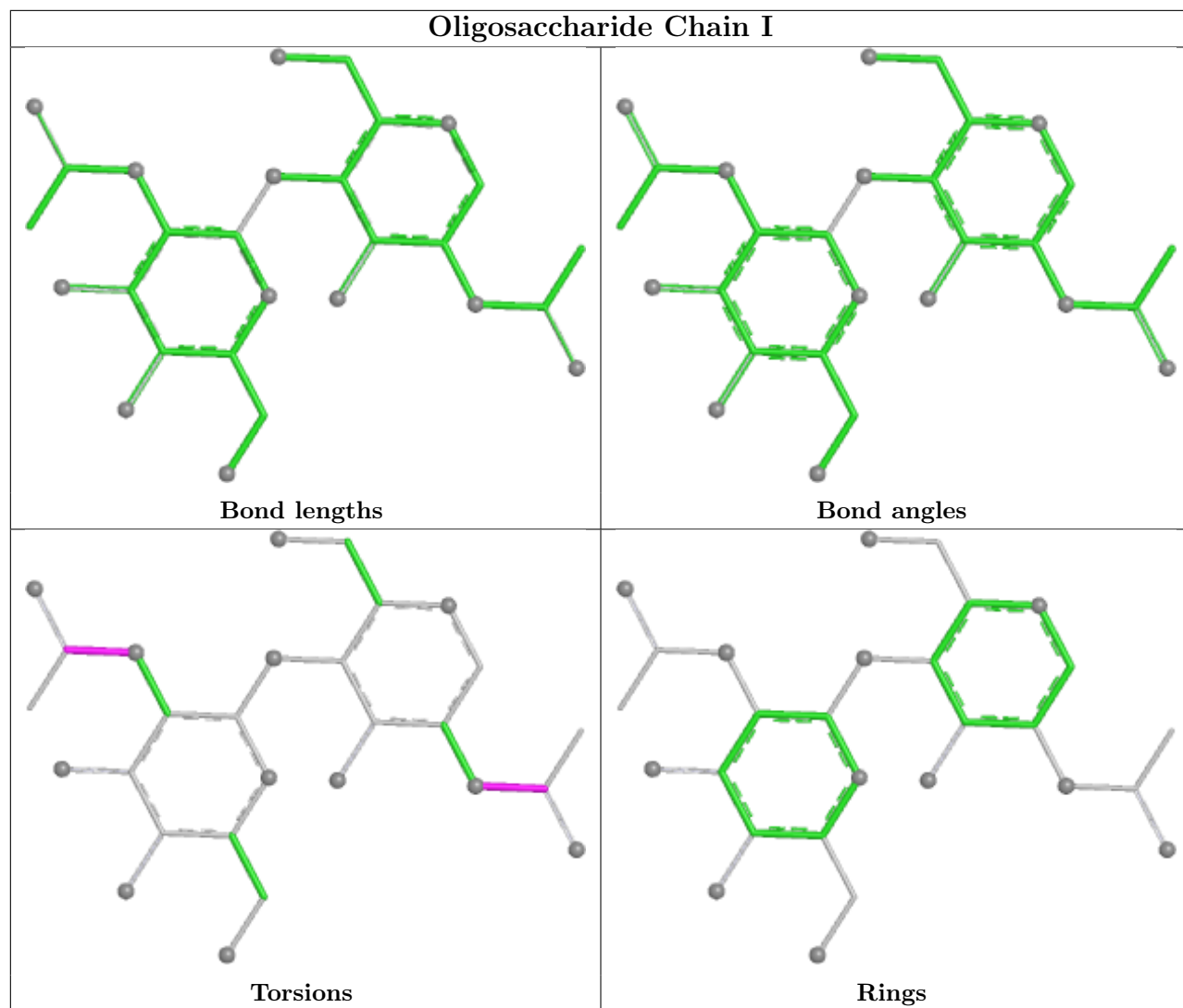
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	2	0
5	E	3	NAG	3	0

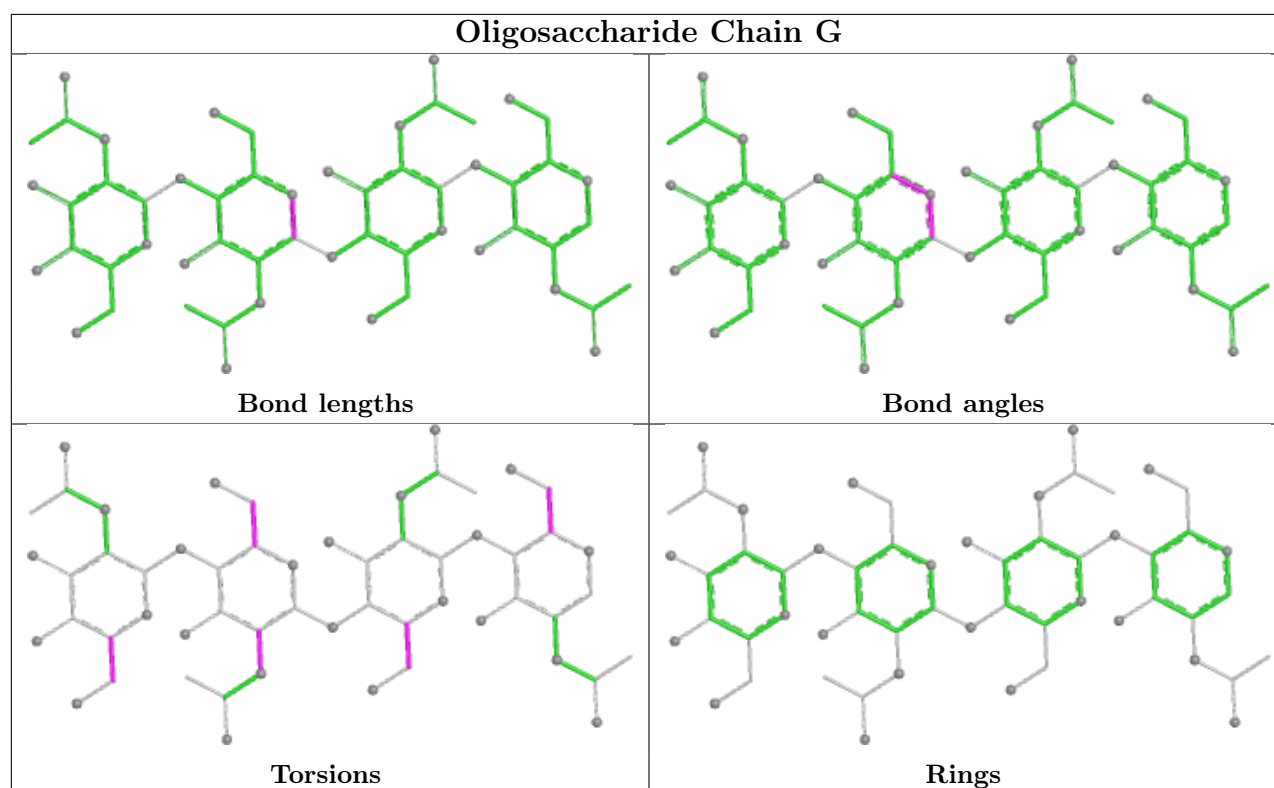
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	NAG	D	1203	2	14,14,15	0.33	0	17,19,21	0.56	0
9	CLR	A	2302	-	31,31,31	0.39	0	48,48,48	0.57	0
9	CLR	A	2303	-	31,31,31	0.39	0	48,48,48	0.64	0
10	NAG	D	1202	2	14,14,15	0.38	0	17,19,21	0.55	0
10	NAG	A	2304	1	14,14,15	0.28	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	D	1203	2	-	0/6/23/26	0/1/1/1
9	CLR	A	2302	-	-	4/10/68/68	0/4/4/4
9	CLR	A	2303	-	-	9/10/68/68	0/4/4/4
10	NAG	D	1202	2	-	4/6/23/26	0/1/1/1
10	NAG	A	2304	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	1202	NAG	O5-C5-C6-O6
10	D	1202	NAG	C4-C5-C6-O6
9	A	2303	CLR	C17-C20-C22-C23
9	A	2303	CLR	C21-C20-C22-C23
9	A	2302	CLR	C20-C22-C23-C24
9	A	2303	CLR	C13-C17-C20-C22
9	A	2303	CLR	C16-C17-C20-C21
9	A	2303	CLR	C22-C23-C24-C25
9	A	2303	CLR	C16-C17-C20-C22
9	A	2303	CLR	C13-C17-C20-C21
9	A	2303	CLR	C23-C24-C25-C27
9	A	2302	CLR	C17-C20-C22-C23
9	A	2303	CLR	C23-C24-C25-C26
10	D	1202	NAG	C3-C2-N2-C7
10	D	1202	NAG	C1-C2-N2-C7
9	A	2302	CLR	C21-C20-C22-C23
9	A	2302	CLR	C22-C23-C24-C25

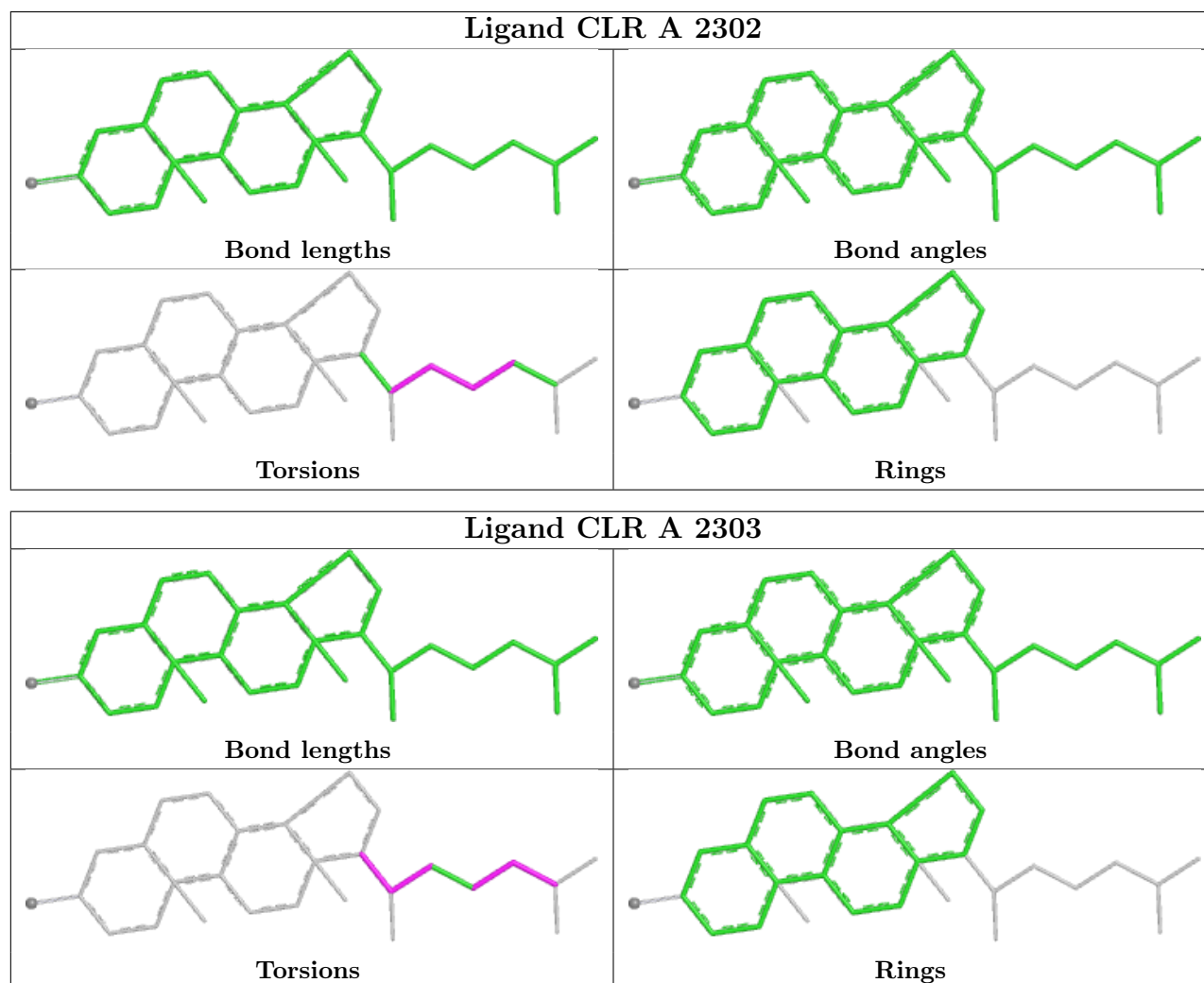
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2302	CLR	3	0
9	A	2303	CLR	6	0
10	D	1202	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.

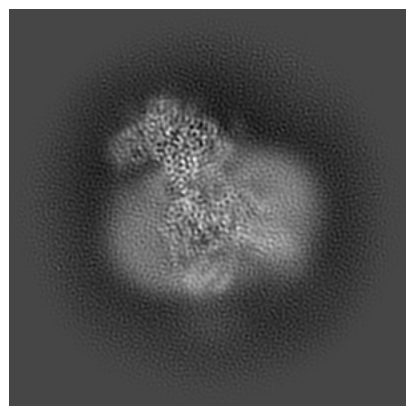
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37473. These allow visual inspection of the internal detail of the map and identification of artifacts.

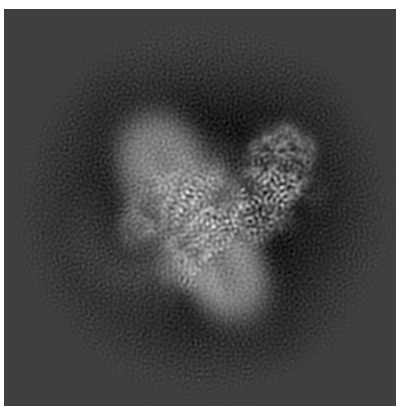
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

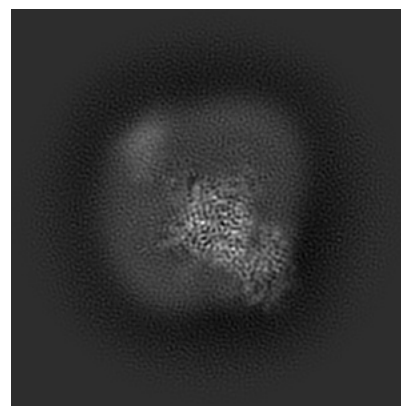
6.1.1 Primary map



X

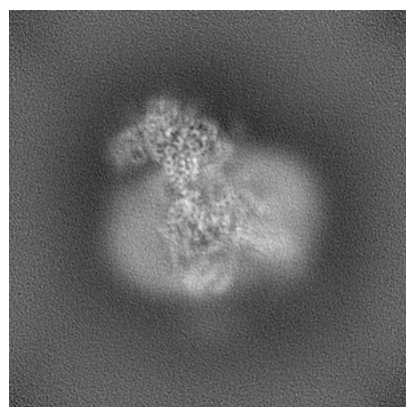


Y

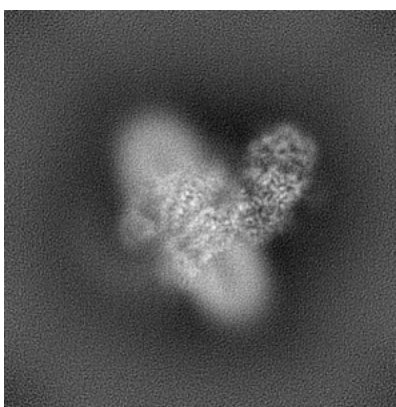


Z

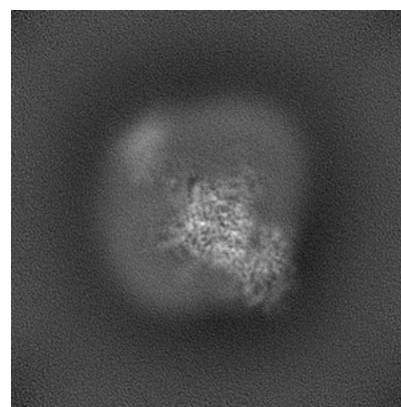
6.1.2 Raw map



X



Y

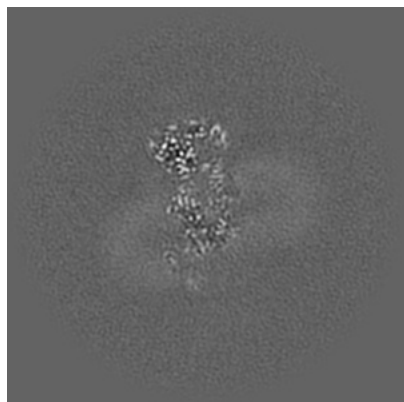


Z

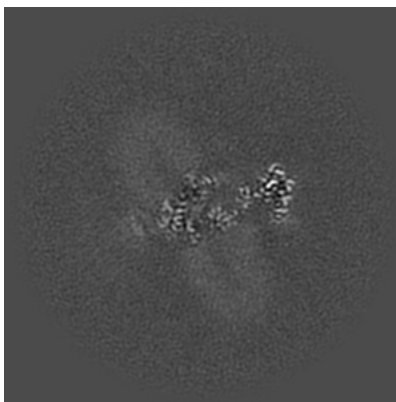
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

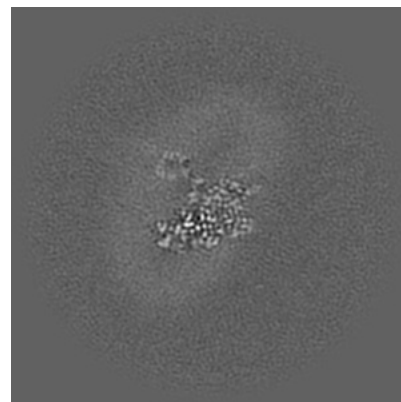
6.2.1 Primary map



X Index: 140

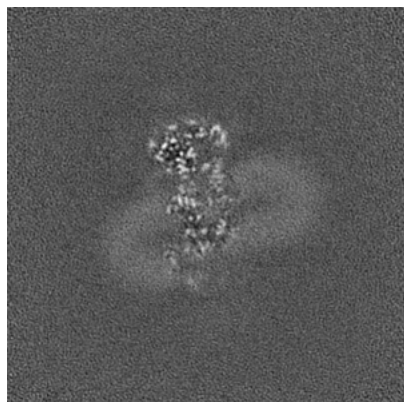


Y Index: 140

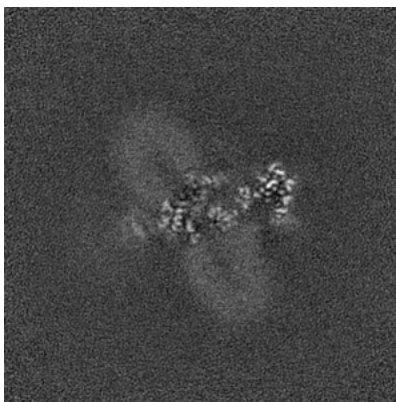


Z Index: 140

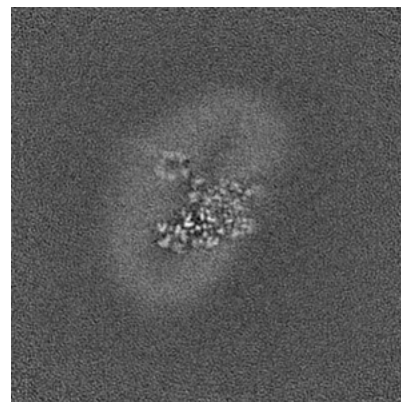
6.2.2 Raw map



X Index: 140



Y Index: 140

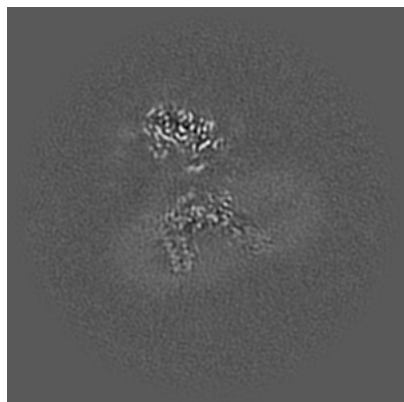


Z Index: 140

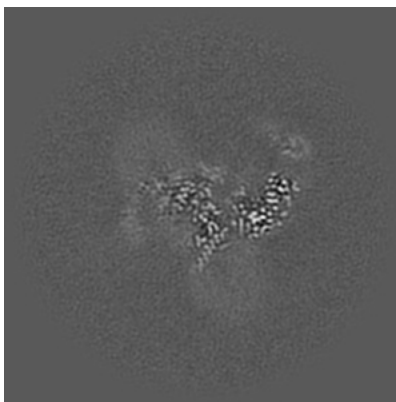
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

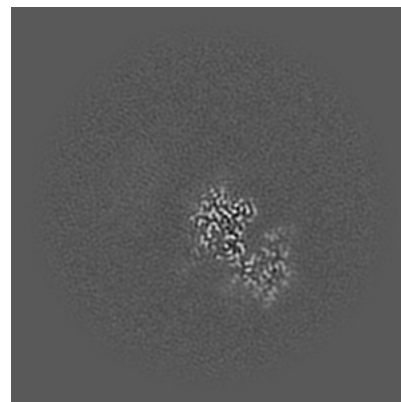
6.3.1 Primary map



X Index: 154

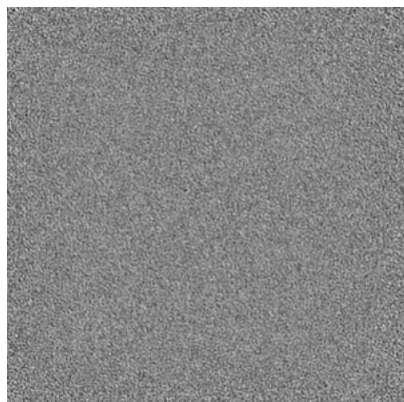


Y Index: 125

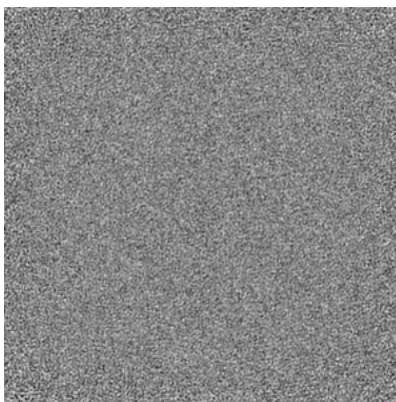


Z Index: 190

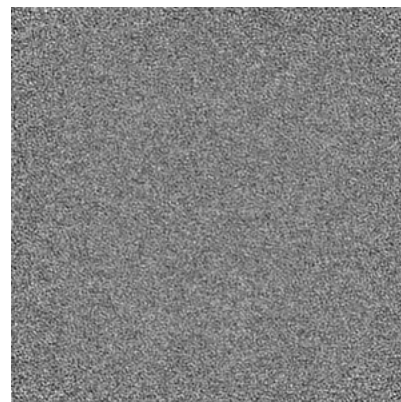
6.3.2 Raw map



X Index: 0



Y Index: 0

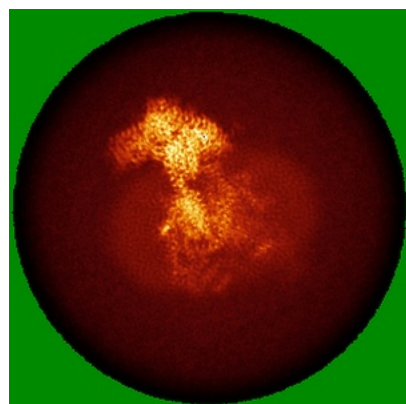


Z Index: 0

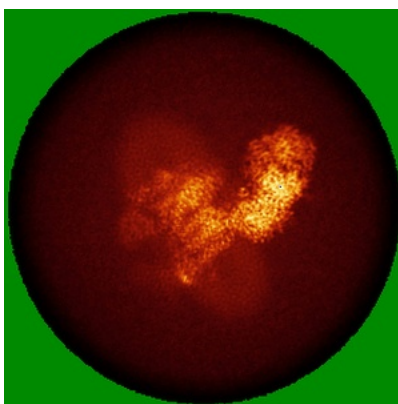
The images above show the largest variance slices of the map in three orthogonal directions.

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

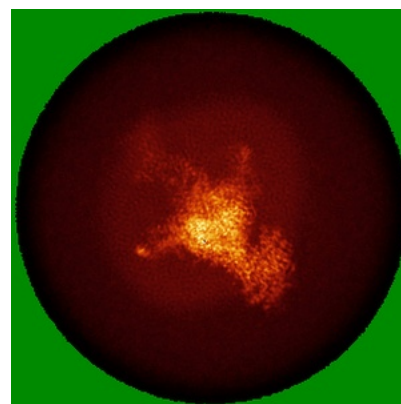
6.4.1 Primary map



X

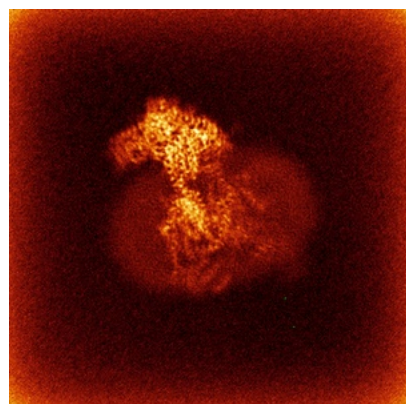


Y

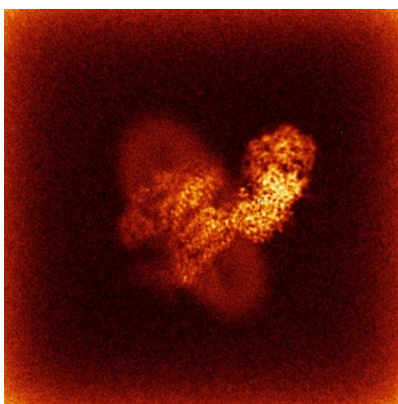


Z

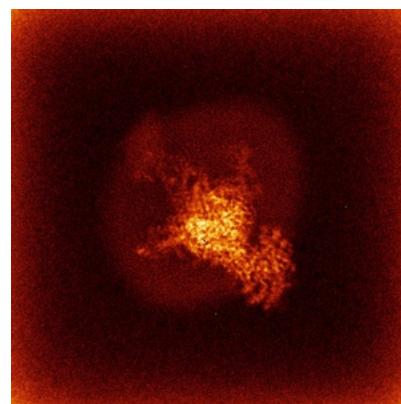
6.4.2 Raw map



X



Y

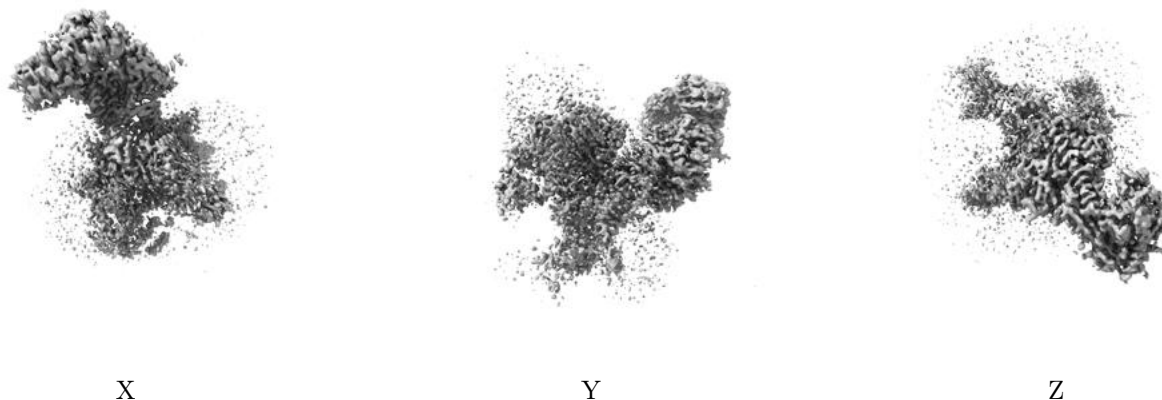


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

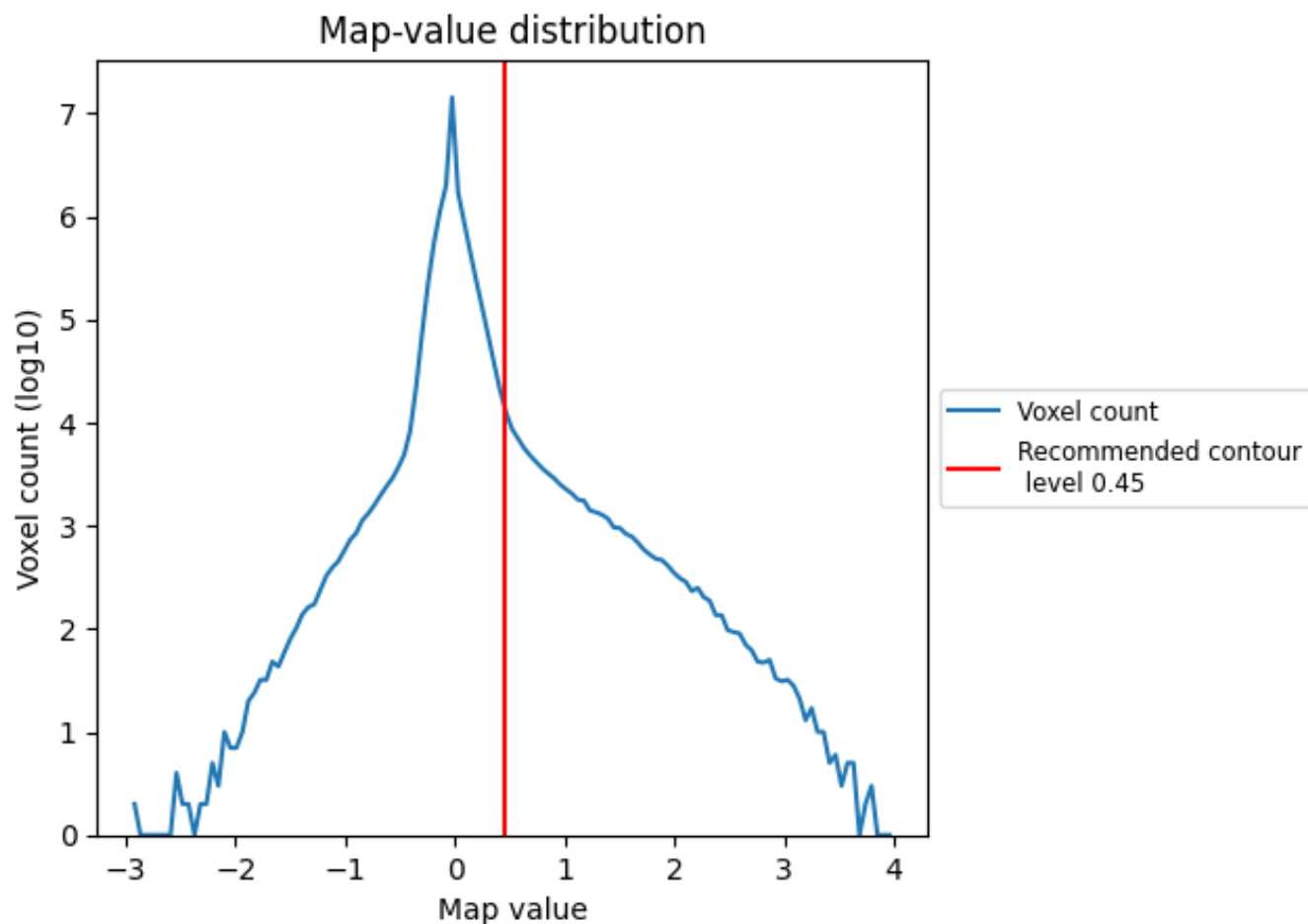
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

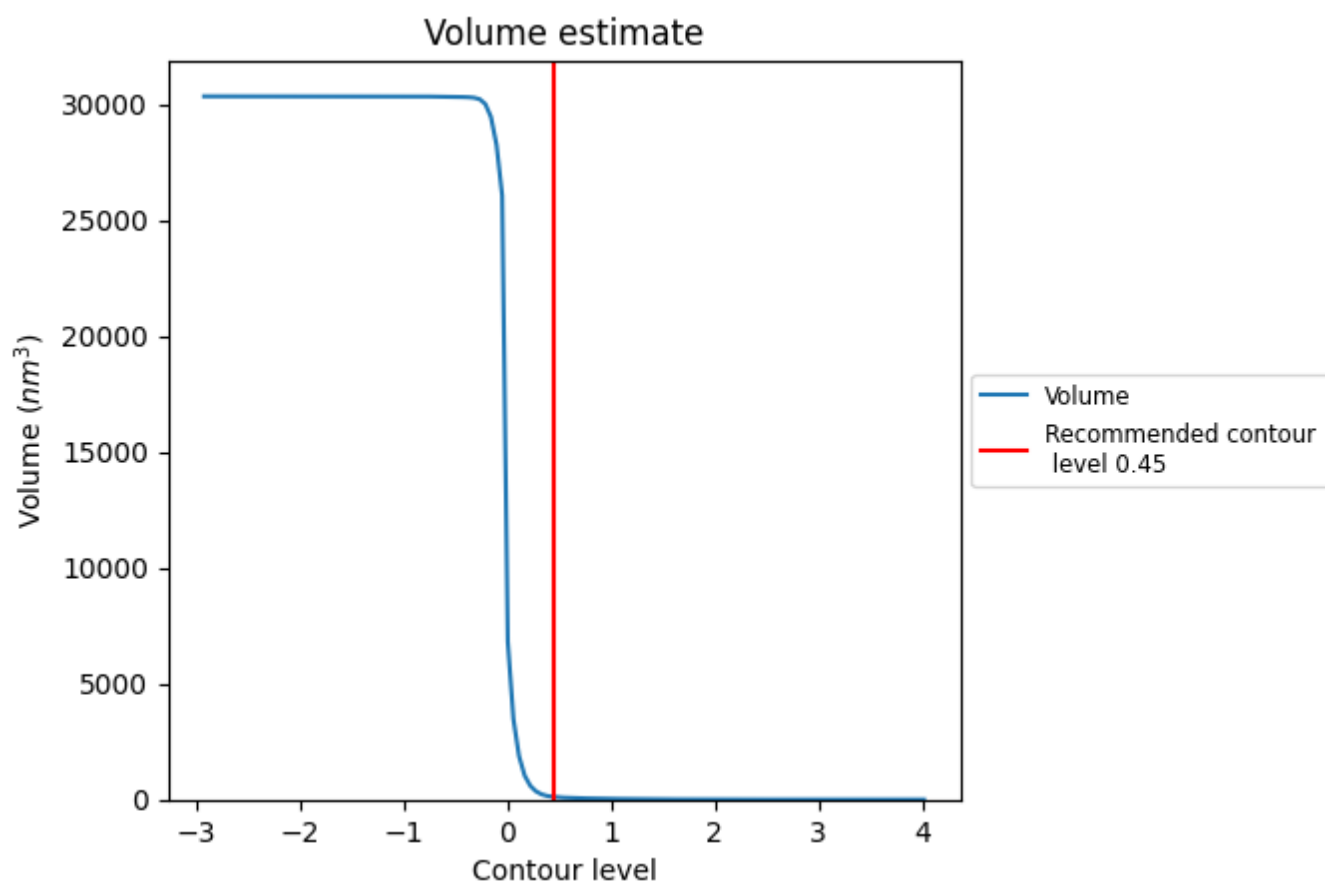
This section contains the results of statistical analysis of the map.

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.

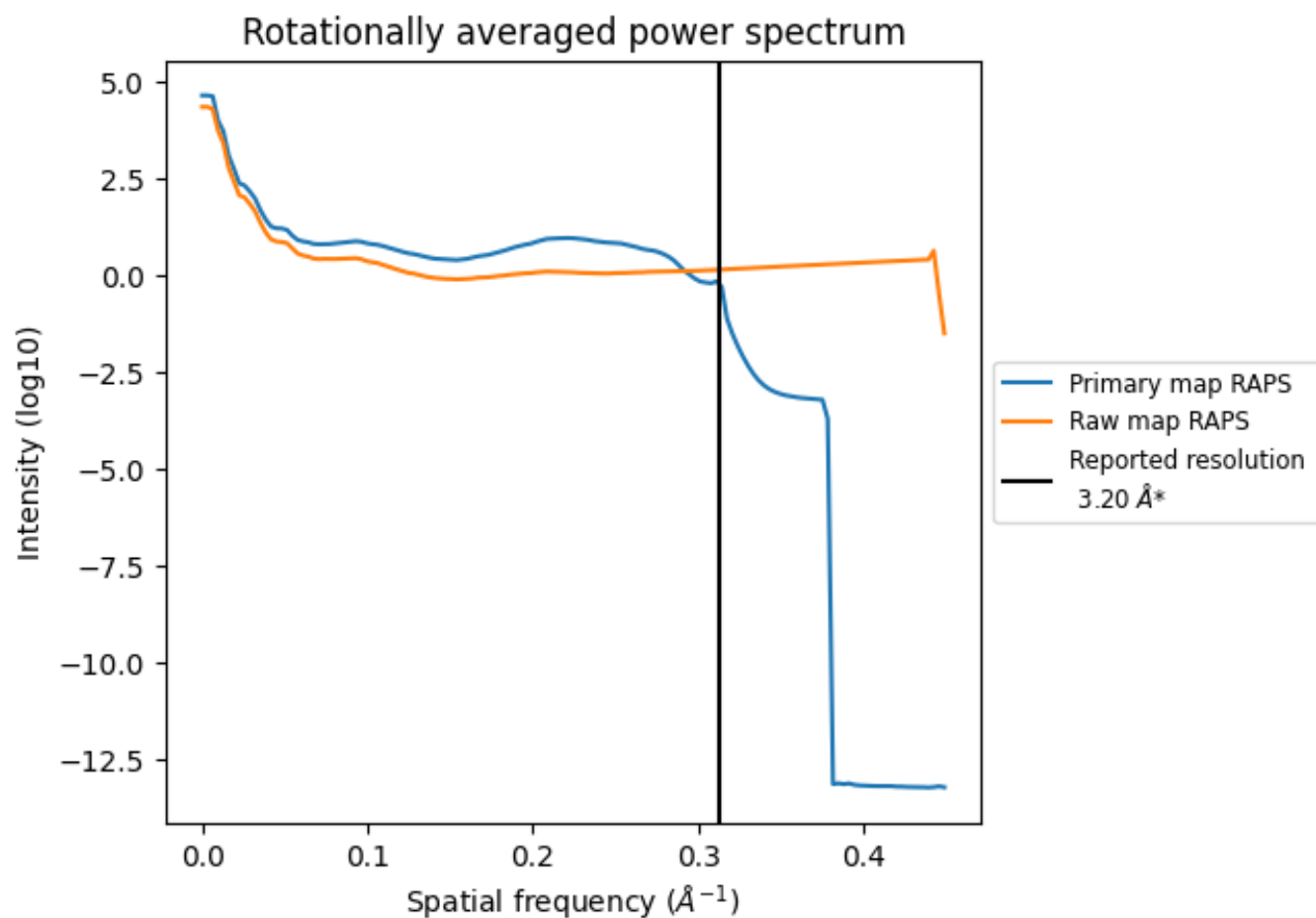
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 103 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 ⓘ

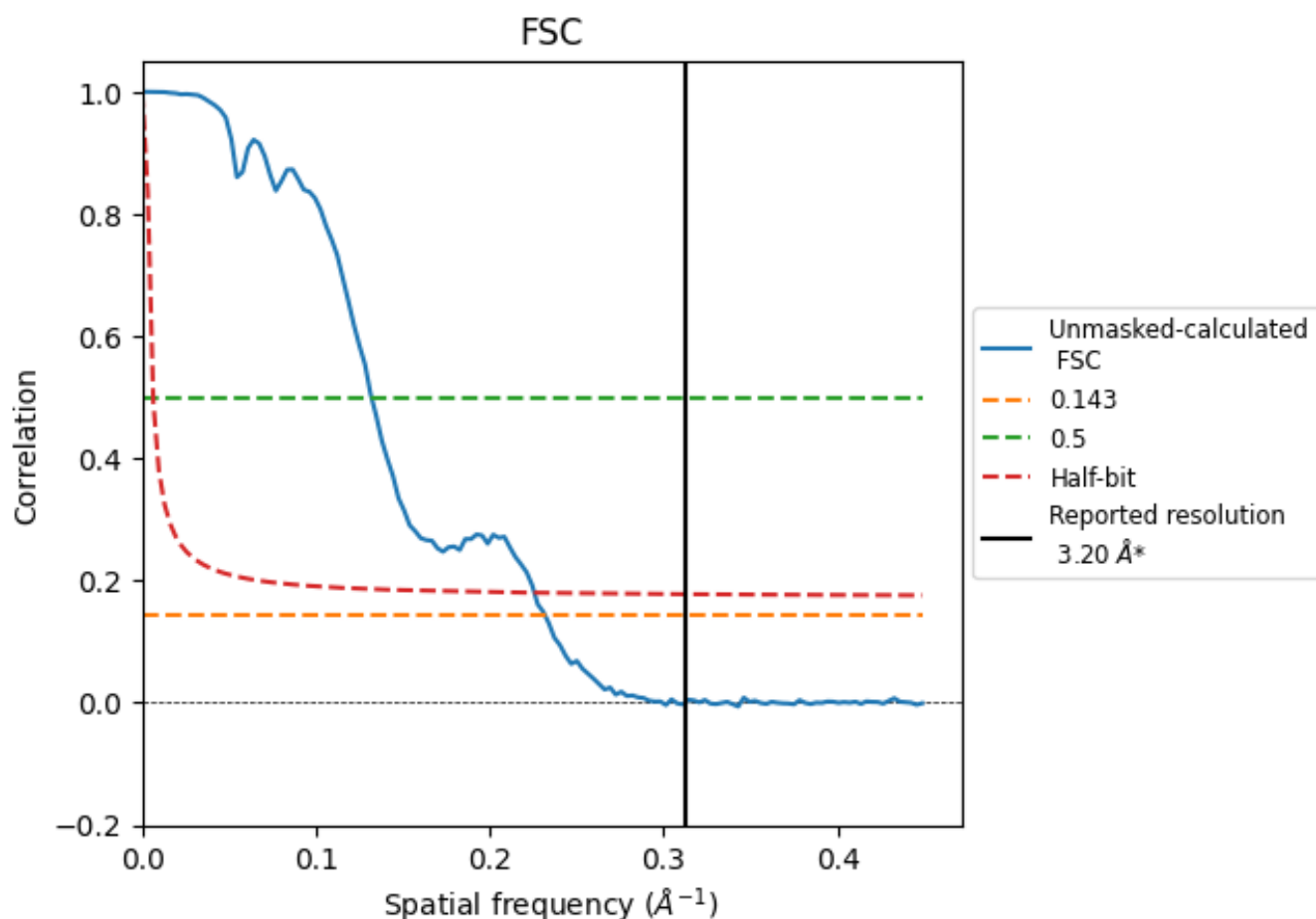


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

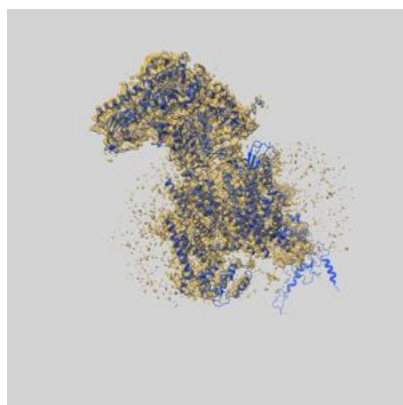
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	7.58	4.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.2 by more than 10 %

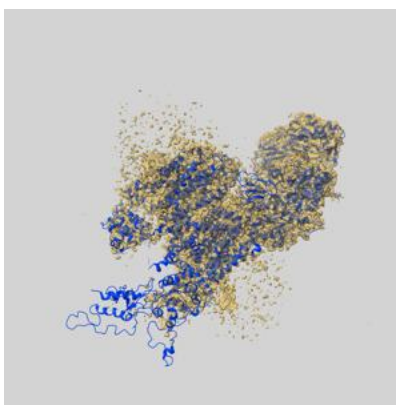
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37473 and PDB model 8WE7. Per-residue inclusion information can be found in section [3](#) on page [8](#).

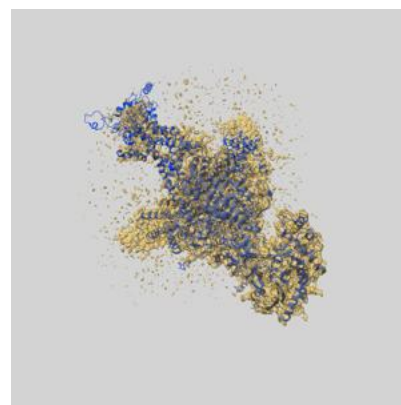
9.1 Map-model overlay [i](#)



X



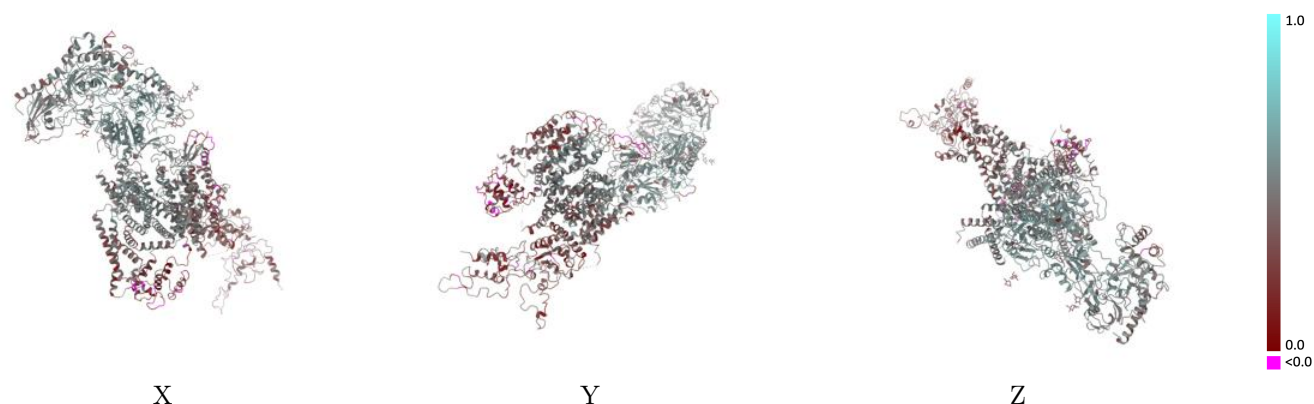
Y



Z

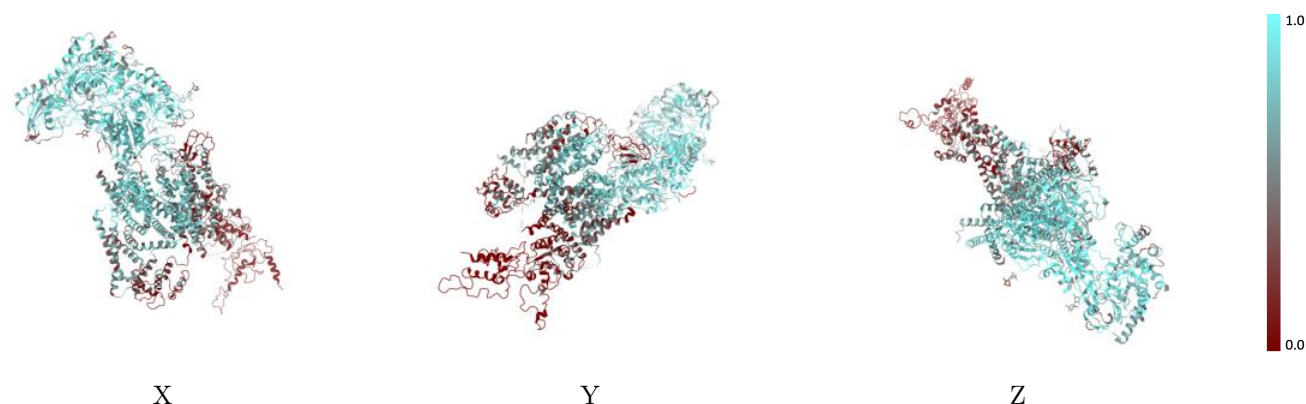
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



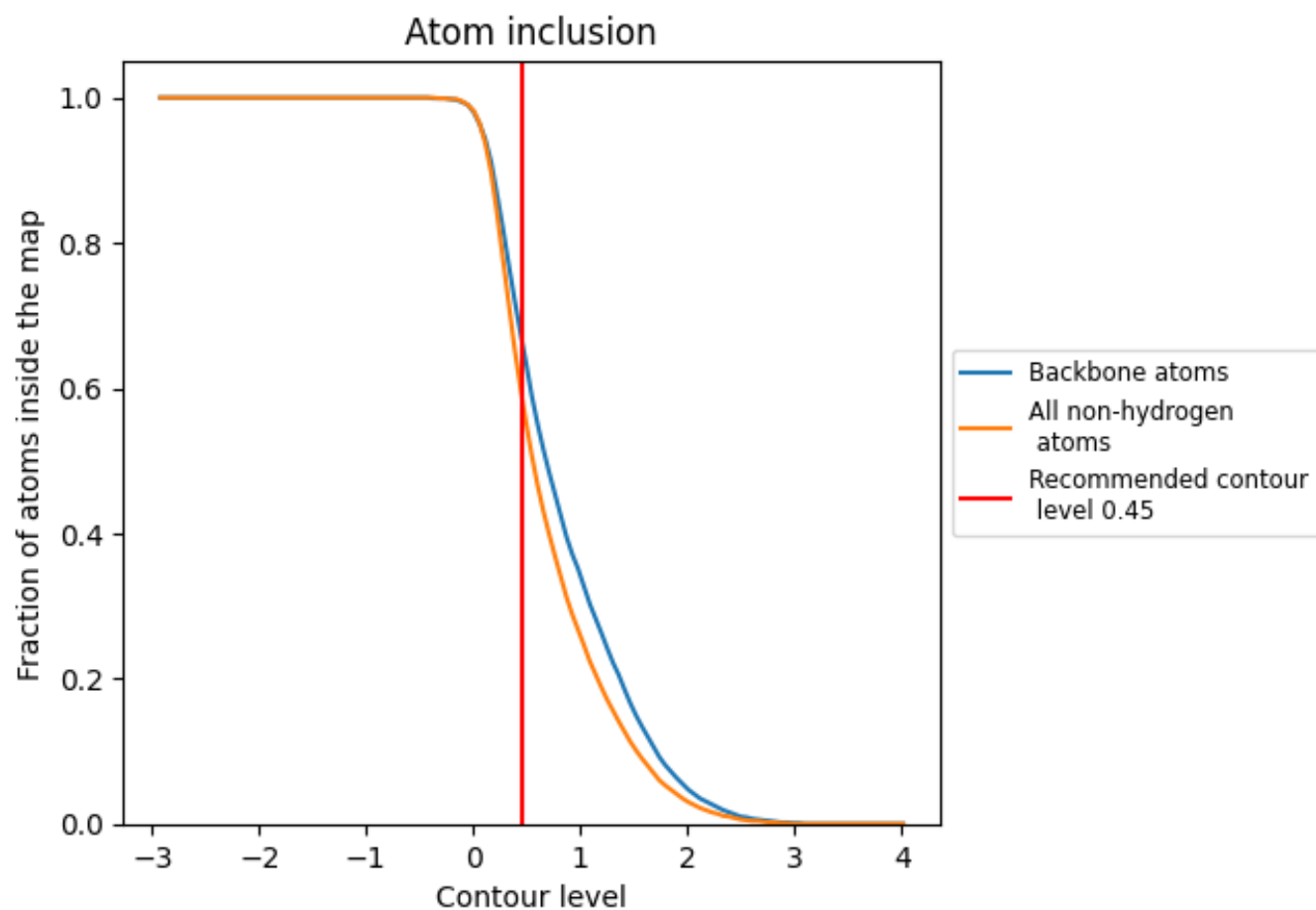
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 59% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5920	0.4360
A	0.5780	0.4170
B	0.1750	0.2790
C	0.0950	0.3240
D	0.8060	0.5110
E	0.5240	0.4020
F	0.2500	0.3130
G	0.6430	0.4270
H	0.6430	0.3950
I	0.5360	0.3220

1.0

0.0

<0.0