Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 08:39 am GMT

PDB ID	:	5A63
EMDB ID	:	EMD-3061
Title	:	Cryo-EM structure of the human gamma-secretase complex at 3.4 angstrom resolution.
Authors	:	Bai, X.; Yan, C.; Yang, G.; Lu, P.; Ma, D.; Sun, L.; Zhou, R.; Scheres, S.H.W.; Shi, Y.
Deposited on	:	2015-06-24
Resolution	:	3.40 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:

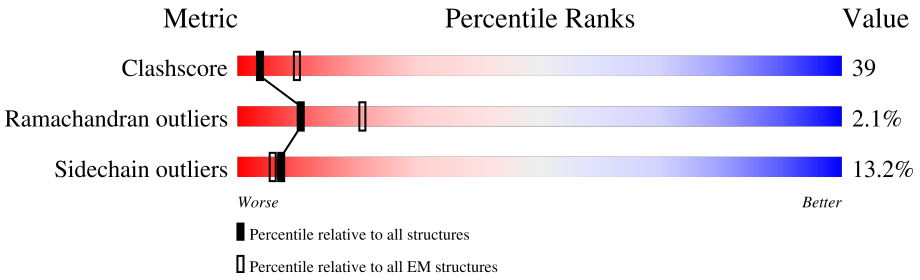
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	709	6% 46% 37% 10% • 6%
2	B	467	7% 28% 15% • 54%
3	C	265	9% 62% 25% 5% 8%
4	D	101	13% 65% 23% 11% •
5	E	2	100%
5	G	2	100%
5	H	2	50% 100%
5	I	2	50% 100%

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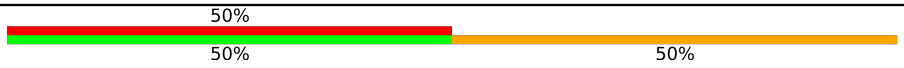
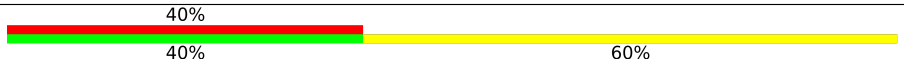
Mol	Chain	Length	Quality of chain
5	J	2	
6	F	5	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10003 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 Nicastrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	665	5222	3312	888	1001	21	0	0

- Molecule 2 is a protein called Presenilin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	215	1702	1170	249	274	9	0	0

- Molecule 3 is a protein called Gamma-secretase subunit APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	243	1872	1254	299	315	4	0	0

- Molecule 4 is a protein called Gamma-secretase subunit PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	100	850	580	134	135	1	0	0

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

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

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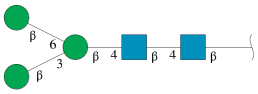
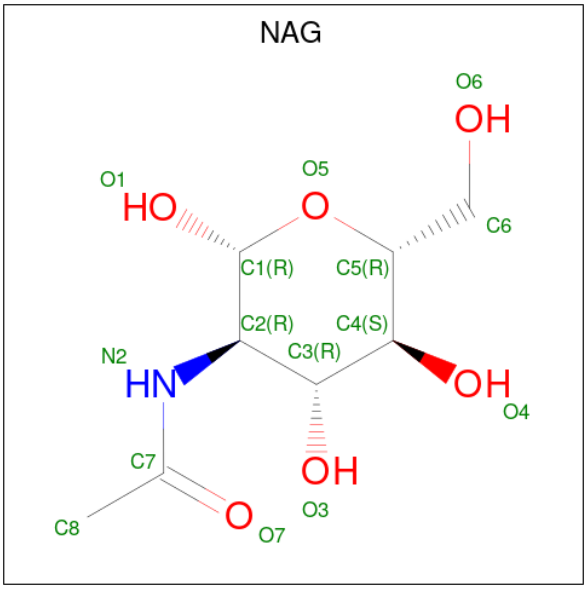
Mol	Chain	Residues	Atoms	AltConf	Trace
5	H	2	Total C N O 28 16 2 10	0	0
5	I	2	Total C N O 28 16 2 10	0	0
5	J	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]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
6	F	5	Total C N O 61 34 2 25	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 70 40 5 25	0

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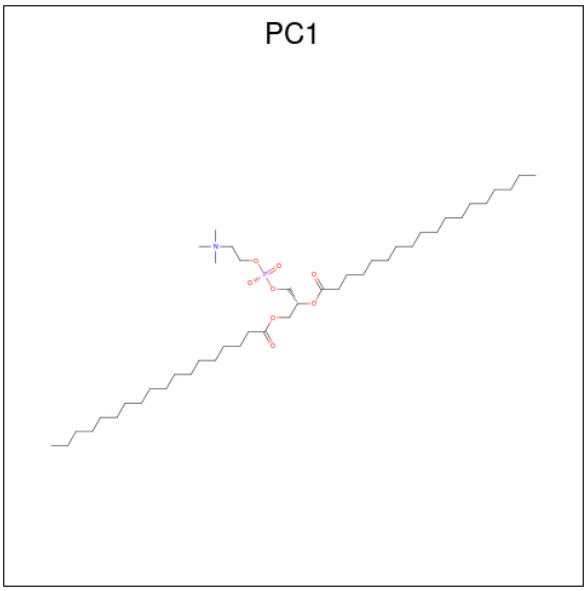
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 70	C 40	N 5	O 25	0
7	A	1	Total 70	C 40	N 5	O 25	0
7	A	1	Total 70	C 40	N 5	O 25	0
7	A	1	Total 70	C 40	N 5	O 25	0

- Molecule 8 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



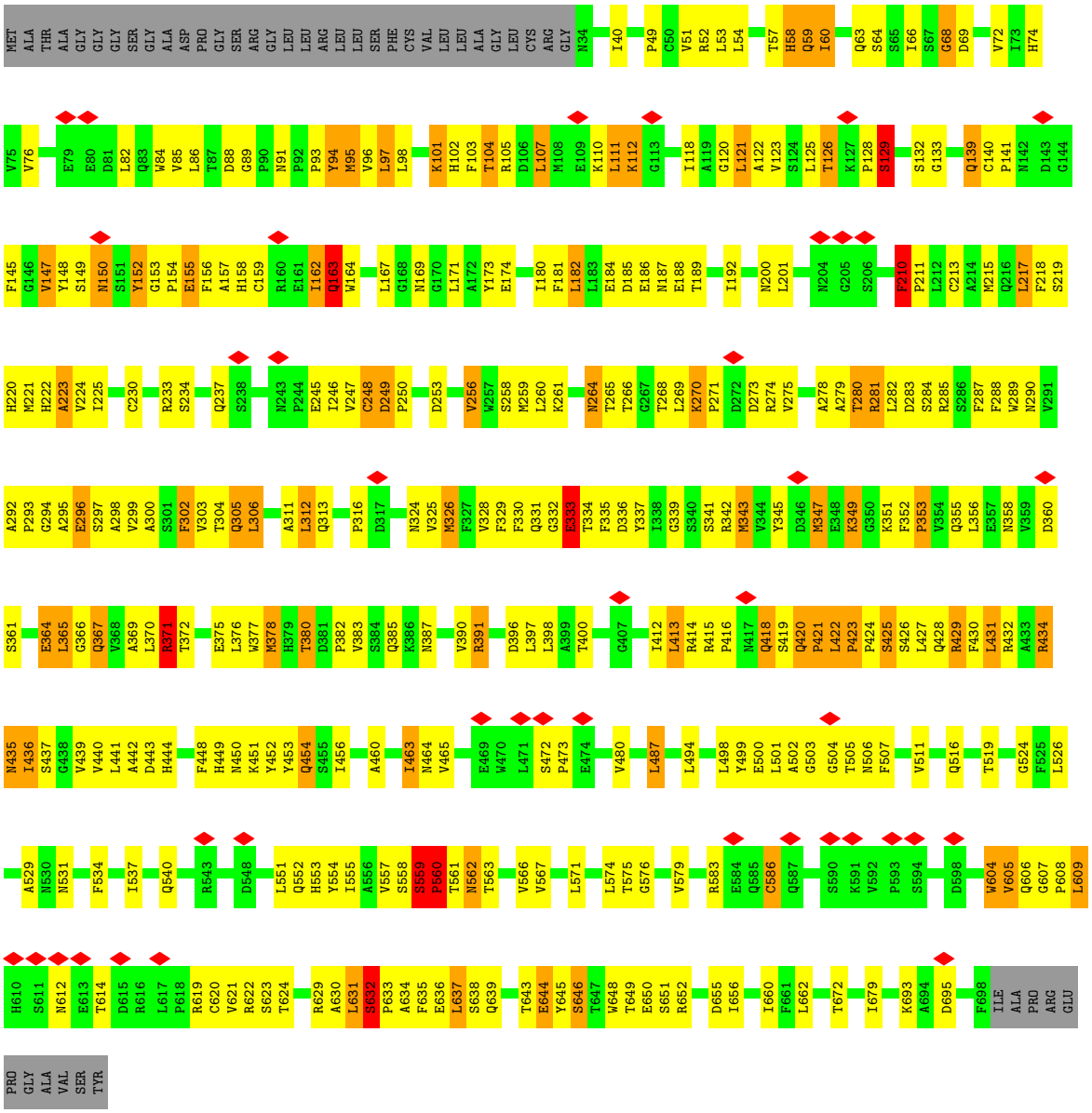
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total 43	C 33	N 1	O 8	P 1	0
8	C	1	Total 43	C 33	N 1	O 8	P 1	0

3 Residue-property plots (i)

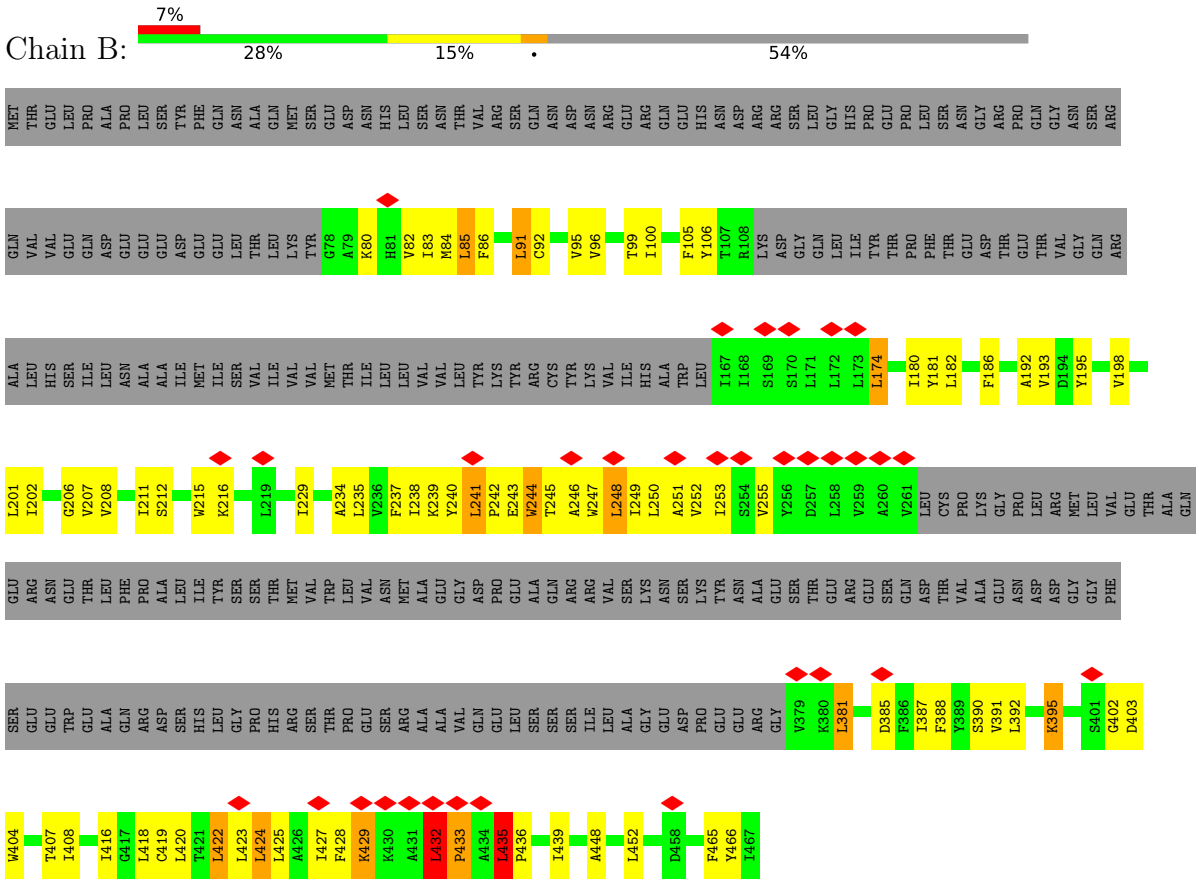
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Nicastrin

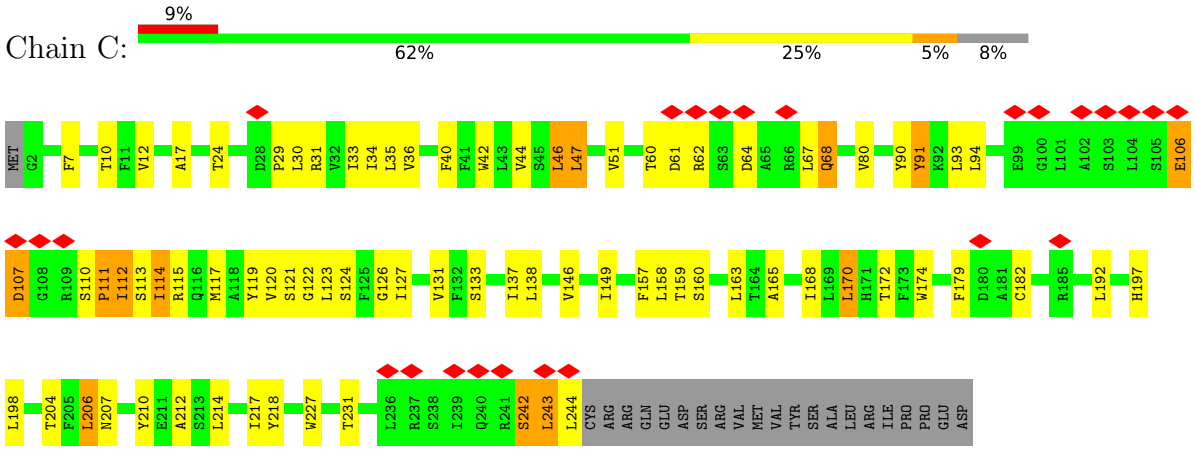
Chain A:



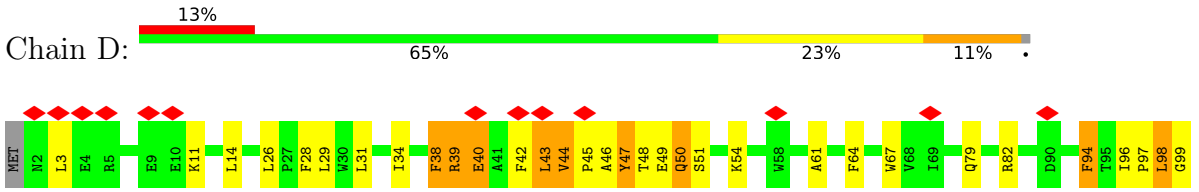
• Molecule 2: Presenilin-1



• Molecule 3: Gamma-secretase subunit APH-1A

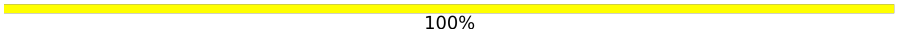


• Molecule 4: Gamma-secretase subunit PEN-2



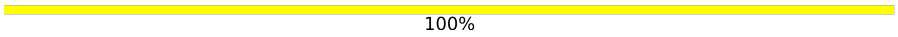
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



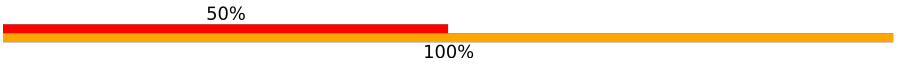
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



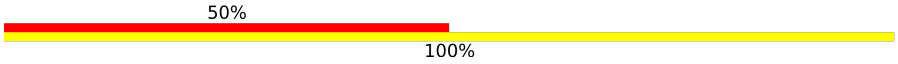
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain I:

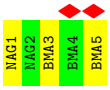


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain F:


NAG1
NAG2
BMA3
BMA4
BMA5

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	159549	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	252.0, 252.0, 252.0	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, PC1, 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	0.54	3/5345 (0.1%)	0.75	8/7284 (0.1%)
2	B	0.46	1/1748 (0.1%)	0.76	1/2385 (0.0%)
3	C	0.48	1/1924 (0.1%)	0.78	1/2624 (0.0%)
4	D	0.53	1/883 (0.1%)	0.74	2/1205 (0.2%)
All	All	0.51	6/9900 (0.1%)	0.76	12/13498 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	N-CD	5.29	1.55	1.47
1	A	608	PRO	N-CD	5.28	1.55	1.47
1	A	421	PRO	N-CD	5.23	1.55	1.47
3	C	111	PRO	N-CD	5.17	1.55	1.47
4	D	101	PRO	N-CD	5.13	1.55	1.47
2	B	433	PRO	N-CD	5.00	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	559	SER	C-N-CD	6.60	142.25	128.40
1	A	423	PRO	C-N-CD	6.05	141.11	128.40
1	A	632	SER	C-N-CD	5.90	140.78	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	422	LEU	C-N-CD	5.81	140.61	128.40
4	D	44	VAL	C-N-CD	5.79	140.57	128.40
4	D	100	THR	C-N-CD	5.75	140.47	128.40
1	A	420	GLN	C-N-CD	5.66	140.28	128.40
3	C	110	SER	C-N-CD	5.57	140.09	128.40
1	A	607	GLY	C-N-CD	5.53	140.01	128.40
1	A	560	PRO	CA-N-CD	-5.37	103.99	111.50
1	A	292	ALA	C-N-CD	5.36	139.65	128.40
2	B	432	LEU	C-N-CD	5.11	139.13	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
1	A	256	VAL	Peptide
1	A	68	GLY	Peptide

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	5222	0	5113	562	0
2	B	1702	0	1793	107	0
3	C	1872	0	1911	88	0
4	D	850	0	840	50	0
5	E	28	0	25	0	0
5	G	28	0	25	0	0
5	H	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	2	0
6	F	61	0	52	0	0
7	A	70	0	65	3	0
8	B	43	0	60	0	0
8	C	43	0	60	1	0
All	All	10003	0	10019	772	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 39.

All (772) 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:316:PRO:HG2	1:A:507:PHE:CD2	1.52	1.42
1:A:152:TYR:CE1	1:A:383:VAL:HG21	1.61	1.36
1:A:279:ALA:O	1:A:364:GLU:HG2	1.29	1.28
1:A:633:PRO:HB2	1:A:645:TYR:CD2	1.66	1.28
1:A:155:GLU:HG3	1:A:156:PHE:CE1	1.71	1.24
1:A:95:MET:CE	1:A:217:LEU:HD11	1.69	1.20
4:D:47:TYR:CB	4:D:50:GLN:HB2	1.72	1.19
4:D:50:GLN:OE1	4:D:54:LYS:HD2	1.43	1.19
1:A:260:LEU:HD22	1:A:312:LEU:HD22	1.23	1.17
1:A:268:THR:CG2	1:A:355:GLN:HG3	1.73	1.17
1:A:156:PHE:CD2	1:A:421:PRO:HB3	1.82	1.14
1:A:223:ALA:HB2	1:A:247:VAL:HG22	1.14	1.13
3:C:34:ILE:HD11	3:C:120:VAL:HB	1.30	1.13
4:D:47:TYR:HB2	4:D:50:GLN:CB	1.79	1.13
1:A:586:CYS:CB	1:A:620:CYS:SG	2.39	1.10
4:D:40:GLU:O	4:D:44:VAL:HG23	1.51	1.10
2:B:82:VAL:HG22	2:B:422:LEU:HD22	1.15	1.09
1:A:316:PRO:CG	1:A:507:PHE:CD2	2.35	1.09
1:A:299:VAL:O	1:A:303:VAL:HG23	1.55	1.07
1:A:604:TRP:HD1	1:A:620:CYS:SG	1.76	1.06
1:A:540:GLN:CG	1:A:606:GLN:HE21	1.68	1.05
1:A:316:PRO:HG2	1:A:507:PHE:CE2	1.92	1.05
1:A:282:LEU:HD13	1:A:329:PHE:HB3	1.08	1.04
1:A:378:MET:HE2	1:A:398:LEU:HD22	1.34	1.04
1:A:249:ASP:HB3	1:A:557:VAL:CG2	1.88	1.04
1:A:311:ALA:O	1:A:511:VAL:HG23	1.55	1.04
1:A:540:GLN:HG2	1:A:606:GLN:NE2	1.73	1.04
1:A:422:LEU:HD23	1:A:423:PRO:HD2	1.38	1.03
1:A:95:MET:HE3	1:A:217:LEU:CD1	1.87	1.02
1:A:378:MET:CE	1:A:398:LEU:HD22	1.88	1.02
1:A:152:TYR:O	1:A:154:PRO:HD3	1.60	1.02
1:A:365:LEU:H	1:A:365:LEU:HD12	1.24	1.02
1:A:432:ARG:HH12	1:A:644:GLU:HB2	1.21	1.02
1:A:95:MET:HE3	1:A:217:LEU:HD11	1.00	1.00
1:A:378:MET:O	1:A:416:PRO:HD3	1.61	1.00
1:A:422:LEU:HD23	1:A:423:PRO:CD	1.90	1.00
1:A:245:GLU:OE2	4:D:98:LEU:HD21	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:PHE:HB3	1:A:421:PRO:HB3	1.40	0.99
1:A:223:ALA:HB2	1:A:247:VAL:CG2	1.91	0.99
1:A:279:ALA:HB2	1:A:328:VAL:CG1	1.93	0.99
1:A:282:LEU:HD23	1:A:331:GLN:NE2	1.77	0.99
1:A:586:CYS:SG	1:A:620:CYS:SG	1.12	0.99
1:A:367:GLN:O	1:A:443:ASP:HB3	1.63	0.98
4:D:44:VAL:HG11	4:D:47:TYR:CD1	1.97	0.98
1:A:152:TYR:CE1	1:A:383:VAL:CG2	2.47	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CD2	1.97	0.98
1:A:250:PRO:HB3	1:A:635:PHE:CE2	1.98	0.98
1:A:280:THR:OG1	1:A:305:GLN:HG2	1.63	0.97
1:A:268:THR:HG23	1:A:355:GLN:HG3	1.40	0.97
1:A:260:LEU:CD2	1:A:312:LEU:HD22	1.94	0.97
1:A:424:PRO:HA	1:A:428:GLN:NE2	1.80	0.97
2:B:429:LYS:H	2:B:429:LYS:HD2	1.30	0.96
1:A:140:CYS:HG	1:A:159:CYS:CB	1.79	0.96
1:A:147:VAL:HG11	1:A:431:LEU:HB3	1.44	0.96
1:A:223:ALA:CB	1:A:247:VAL:HG22	1.97	0.95
1:A:633:PRO:CB	1:A:645:TYR:HD2	1.78	0.95
2:B:244:TRP:CE3	2:B:247:TRP:HD1	1.84	0.95
1:A:249:ASP:HB3	1:A:557:VAL:HG21	1.48	0.94
1:A:230:CYS:SG	1:A:247:VAL:HG13	2.06	0.94
1:A:268:THR:HG21	1:A:355:GLN:HG3	1.50	0.93
1:A:224:VAL:HG21	4:D:101:PRO:HA	1.49	0.93
1:A:152:TYR:HE1	1:A:383:VAL:CG2	1.79	0.93
1:A:311:ALA:C	1:A:511:VAL:HG23	1.89	0.93
1:A:281:ARG:HG3	1:A:281:ARG:HH11	1.35	0.92
3:C:34:ILE:HD11	3:C:120:VAL:CB	1.99	0.92
1:A:152:TYR:HE1	1:A:383:VAL:HG21	1.10	0.92
1:A:139:GLN:HG2	1:A:163:GLN:HG2	1.51	0.92
3:C:90:TYR:CE2	3:C:94:LEU:HD11	2.05	0.91
1:A:279:ALA:CB	1:A:328:VAL:CG1	2.49	0.91
1:A:633:PRO:HB2	1:A:645:TYR:HD2	1.04	0.90
1:A:224:VAL:CG2	4:D:101:PRO:HA	2.02	0.89
1:A:540:GLN:HG2	1:A:606:GLN:HE21	1.33	0.89
1:A:622:ARG:HG2	1:A:622:ARG:HH11	1.35	0.89
1:A:397:LEU:CD2	1:A:439:VAL:HG23	2.02	0.89
1:A:156:PHE:CB	1:A:421:PRO:HB3	2.02	0.89
2:B:239:LYS:CG	2:B:240:TYR:CE1	2.55	0.89
1:A:300:ALA:O	1:A:304:THR:HG23	1.71	0.89
1:A:152:TYR:HD1	1:A:153:GLY:N	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:CD1	1:A:329:PHE:HB3	1.99	0.88
1:A:156:PHE:CG	1:A:421:PRO:HB3	2.08	0.88
1:A:224:VAL:HG21	4:D:100:THR:O	1.73	0.87
1:A:633:PRO:CB	1:A:645:TYR:CD2	2.51	0.87
1:A:586:CYS:SG	1:A:620:CYS:CB	2.62	0.87
2:B:82:VAL:HG22	2:B:422:LEU:CD2	2.03	0.87
1:A:249:ASP:CB	1:A:557:VAL:HG21	2.04	0.87
1:A:316:PRO:HG2	1:A:507:PHE:HD2	1.05	0.87
1:A:361:SER:OG	1:A:501:LEU:HD13	1.74	0.87
2:B:239:LYS:HG2	2:B:240:TYR:CE1	2.10	0.87
1:A:152:TYR:CZ	1:A:383:VAL:HG11	2.10	0.86
1:A:96:VAL:HG22	1:A:118:ILE:HD11	1.57	0.86
1:A:604:TRP:CD1	1:A:620:CYS:SG	2.66	0.86
1:A:162:ILE:HG21	1:A:420:GLN:OE1	1.74	0.85
1:A:156:PHE:HD2	1:A:421:PRO:HB3	1.39	0.85
1:A:371:ARG:CB	1:A:371:ARG:HH11	1.88	0.85
1:A:156:PHE:HB3	1:A:421:PRO:CB	2.06	0.85
1:A:156:PHE:CD2	1:A:421:PRO:CB	2.59	0.85
1:A:279:ALA:HB1	1:A:330:PHE:CE2	2.11	0.84
1:A:260:LEU:HD22	1:A:312:LEU:CD2	2.05	0.84
1:A:635:PHE:HZ	1:A:649:THR:HG23	1.43	0.84
1:A:155:GLU:HG3	1:A:156:PHE:CD1	2.13	0.83
1:A:378:MET:CE	1:A:398:LEU:CD2	2.55	0.83
1:A:140:CYS:SG	1:A:159:CYS:HB3	2.19	0.83
1:A:451:LYS:HB2	1:A:451:LYS:NZ	1.94	0.83
1:A:259:MET:SD	1:A:326:MET:CB	2.66	0.83
1:A:259:MET:SD	1:A:326:MET:HB2	2.19	0.83
1:A:260:LEU:CD2	1:A:312:LEU:CD2	2.56	0.83
2:B:86:PHE:CZ	2:B:419:CYS:SG	2.71	0.83
1:A:128:PRO:O	1:A:129:SER:HB2	1.78	0.83
2:B:198:VAL:HG21	4:D:94:PHE:CE1	2.14	0.82
4:D:3:LEU:HD23	4:D:40:GLU:OE1	1.79	0.82
1:A:268:THR:HG21	1:A:355:GLN:CG	2.10	0.82
1:A:563:THR:O	1:A:567:VAL:HG23	1.78	0.82
1:A:418:GLN:HE21	1:A:419:SER:H	1.28	0.82
1:A:540:GLN:HG3	1:A:606:GLN:HE21	1.42	0.82
2:B:245:THR:O	2:B:249:ILE:HG13	1.80	0.82
1:A:279:ALA:HB1	1:A:330:PHE:HE2	1.45	0.81
3:C:17:ALA:HB2	3:C:168:ILE:HG21	1.62	0.81
1:A:324:ASN:OD1	1:A:325:VAL:N	2.12	0.81
2:B:243:GLU:O	2:B:247:TRP:CD1	2.33	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLY:HA2	1:A:218:PHE:CD1	2.16	0.81
2:B:96:VAL:HG21	2:B:390:SER:HB3	1.62	0.81
1:A:279:ALA:CB	1:A:328:VAL:HG13	2.11	0.81
1:A:311:ALA:O	1:A:511:VAL:CG2	2.28	0.81
1:A:299:VAL:CG2	1:A:553:HIS:NE2	2.44	0.80
2:B:244:TRP:CZ3	2:B:247:TRP:HD1	2.00	0.80
1:A:586:CYS:HG	1:A:620:CYS:CB	1.91	0.80
1:A:147:VAL:CG1	1:A:431:LEU:HB3	2.12	0.80
1:A:397:LEU:HD23	1:A:439:VAL:HG23	1.64	0.80
1:A:316:PRO:CG	1:A:507:PHE:HD2	1.82	0.79
1:A:378:MET:HE2	1:A:398:LEU:CD2	2.12	0.79
1:A:68:GLY:CA	1:A:218:PHE:CE1	2.66	0.79
1:A:432:ARG:NH1	1:A:644:GLU:HB2	1.97	0.78
1:A:96:VAL:HG23	1:A:121:LEU:HB3	1.66	0.78
2:B:99:THR:HG21	2:B:181:TYR:HE1	1.49	0.78
1:A:280:THR:OG1	1:A:305:GLN:CG	2.30	0.78
1:A:245:GLU:OE2	4:D:98:LEU:CD2	2.31	0.77
2:B:244:TRP:CZ3	2:B:247:TRP:CD1	2.72	0.77
1:A:343:MET:O	1:A:347:MET:HG2	1.84	0.77
1:A:281:ARG:HG3	1:A:281:ARG:NH1	1.98	0.77
1:A:605:VAL:CG1	1:A:621:VAL:HG23	2.15	0.76
2:B:435:LEU:H	2:B:436:PRO:HD3	1.50	0.76
1:A:152:TYR:CD1	1:A:153:GLY:N	2.53	0.76
3:C:60:THR:HG21	3:C:67:LEU:HD21	1.67	0.76
1:A:269:LEU:HB3	1:A:358:ASN:HD21	1.48	0.76
2:B:237:PHE:O	2:B:241:LEU:HB2	1.85	0.76
2:B:435:LEU:CD1	2:B:439:ILE:CD1	2.64	0.76
1:A:223:ALA:CA	1:A:247:VAL:HG21	2.17	0.75
2:B:448:ALA:HB1	3:C:47:LEU:HD21	1.68	0.75
1:A:250:PRO:HA	1:A:649:THR:HG22	1.67	0.75
1:A:311:ALA:C	1:A:511:VAL:CG2	2.56	0.74
1:A:635:PHE:CZ	1:A:649:THR:HG23	2.22	0.74
2:B:239:LYS:HG3	2:B:240:TYR:CE1	2.23	0.74
1:A:279:ALA:O	1:A:364:GLU:CG	2.24	0.74
1:A:637:LEU:CB	1:A:639:GLN:HE21	2.01	0.73
4:D:47:TYR:HB2	4:D:50:GLN:HB2	0.83	0.73
1:A:64:SER:CB	1:A:219:SER:H	2.01	0.73
1:A:637:LEU:HB3	1:A:639:GLN:HE21	1.52	0.73
1:A:139:GLN:CG	1:A:163:GLN:HG2	2.18	0.73
1:A:269:LEU:HB3	1:A:358:ASN:ND2	2.04	0.73
2:B:85:LEU:HD22	2:B:418:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:LEU:N	2:B:436:PRO:CD	2.52	0.73
2:B:435:LEU:HD12	2:B:439:ILE:HG13	1.70	0.73
2:B:429:LYS:HD2	2:B:429:LYS:N	2.03	0.73
1:A:397:LEU:HG	1:A:439:VAL:HG21	1.69	0.73
1:A:282:LEU:HD13	1:A:329:PHE:CB	2.04	0.72
1:A:299:VAL:HG22	1:A:553:HIS:NE2	2.04	0.72
1:A:633:PRO:HB2	1:A:645:TYR:CE2	2.23	0.72
1:A:266:THR:HB	7:A:1714:NAG:O7	1.88	0.72
1:A:418:GLN:HE21	1:A:419:SER:N	1.87	0.72
1:A:152:TYR:C	1:A:154:PRO:HD3	2.10	0.72
2:B:241:LEU:HG	2:B:245:THR:HG22	1.70	0.72
1:A:418:GLN:HE21	1:A:418:GLN:CA	2.03	0.72
2:B:174:LEU:HG	2:B:229:ILE:HD11	1.71	0.72
1:A:422:LEU:HD23	1:A:423:PRO:N	2.03	0.72
1:A:140:CYS:SG	1:A:159:CYS:CB	2.74	0.72
1:A:418:GLN:NE2	1:A:419:SER:H	1.86	0.72
1:A:259:MET:SD	1:A:326:MET:HB3	2.30	0.71
1:A:95:MET:CE	1:A:217:LEU:CD1	2.59	0.71
1:A:504:GLY:O	1:A:505:THR:OG1	2.08	0.71
3:C:112:ILE:HD13	3:C:112:ILE:H	1.56	0.71
1:A:290:ASN:O	1:A:552:GLN:HG3	1.88	0.71
1:A:299:VAL:O	1:A:303:VAL:CG2	2.34	0.71
1:A:224:VAL:HG21	4:D:101:PRO:CA	2.20	0.71
1:A:64:SER:HB3	1:A:219:SER:H	1.56	0.70
2:B:239:LYS:CG	2:B:240:TYR:HE1	2.01	0.70
1:A:253:ASP:HB3	1:A:559:SER:O	1.91	0.70
1:A:261:LYS:O	1:A:324:ASN:ND2	2.24	0.70
1:A:451:LYS:HB2	1:A:451:LYS:HZ2	1.55	0.70
1:A:249:ASP:HB3	1:A:557:VAL:HG23	1.73	0.70
1:A:95:MET:HE2	1:A:215:MET:HE3	1.74	0.70
1:A:279:ALA:CB	1:A:330:PHE:HE2	2.05	0.70
1:A:367:GLN:O	1:A:443:ASP:CB	2.38	0.70
3:C:34:ILE:CG1	3:C:120:VAL:HG11	2.21	0.69
1:A:133:GLY:HA2	1:A:452:TYR:HE1	1.56	0.69
1:A:171:LEU:HD23	1:A:287:PHE:CE2	2.26	0.69
1:A:66:ILE:HD13	1:A:220:HIS:ND1	2.07	0.69
1:A:316:PRO:CG	1:A:507:PHE:CE2	2.72	0.69
1:A:150:ASN:O	1:A:154:PRO:HG3	1.91	0.69
1:A:424:PRO:HA	1:A:428:GLN:HE22	1.57	0.69
1:A:279:ALA:HB2	1:A:328:VAL:HG11	1.73	0.69
2:B:239:LYS:HG2	2:B:240:TYR:HE1	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:LEU:HG	4:D:11:LYS:HE2	1.75	0.69
1:A:233:ARG:O	1:A:237:GLN:HG2	1.92	0.69
1:A:278:ALA:C	1:A:305:GLN:HE22	1.97	0.69
1:A:397:LEU:CD2	1:A:439:VAL:CG2	2.71	0.69
1:A:164:TRP:CE2	1:A:423:PRO:HA	2.28	0.68
1:A:372:THR:HG23	1:A:449:HIS:CD2	2.28	0.68
1:A:95:MET:CE	1:A:215:MET:CE	2.70	0.68
1:A:94:TYR:O	1:A:118:ILE:HG13	1.94	0.68
1:A:95:MET:HG2	1:A:120:GLY:O	1.94	0.68
1:A:223:ALA:N	1:A:247:VAL:CG2	2.57	0.68
1:A:300:ALA:HB2	1:A:463:ILE:HD12	1.76	0.68
1:A:311:ALA:HB1	1:A:511:VAL:CG2	2.24	0.68
1:A:171:LEU:HD23	1:A:287:PHE:HE2	1.59	0.68
1:A:300:ALA:HB1	1:A:369:ALA:HB2	1.76	0.68
1:A:633:PRO:O	1:A:637:LEU:HD22	1.94	0.68
3:C:179:PHE:O	3:C:182:CYS:SG	2.52	0.68
1:A:141:PRO:HG2	1:A:424:PRO:HG3	1.75	0.68
1:A:223:ALA:CA	1:A:247:VAL:CG2	2.72	0.68
1:A:256:VAL:HG22	1:A:329:PHE:HB2	1.76	0.68
1:A:68:GLY:N	1:A:218:PHE:CD1	2.62	0.67
1:A:96:VAL:HG23	1:A:121:LEU:CB	2.24	0.67
1:A:111:LEU:HD21	1:A:118:ILE:HD13	1.76	0.67
1:A:95:MET:CE	1:A:215:MET:HE2	2.24	0.67
1:A:311:ALA:HB1	1:A:511:VAL:HG22	1.76	0.67
1:A:281:ARG:HB2	1:A:333:GLU:HB2	1.75	0.67
1:A:68:GLY:N	1:A:218:PHE:CE1	2.63	0.67
1:A:453:TYR:O	1:A:454:GLN:C	2.32	0.67
2:B:182:LEU:HD21	2:B:201:LEU:HD23	1.76	0.67
1:A:54:LEU:HD12	1:A:248:CYS:SG	2.35	0.67
2:B:435:LEU:HD11	2:B:439:ILE:CD1	2.24	0.67
3:C:163:LEU:HD11	3:C:217:ILE:HD13	1.75	0.67
1:A:72:VAL:HG13	1:A:94:TYR:CD1	2.29	0.67
1:A:256:VAL:HG21	1:A:567:VAL:HG12	1.77	0.67
1:A:605:VAL:HG11	1:A:621:VAL:CG2	2.24	0.67
1:A:64:SER:N	1:A:219:SER:O	2.28	0.67
1:A:224:VAL:HG11	4:D:99:GLY:O	1.94	0.66
2:B:435:LEU:CD1	2:B:439:ILE:HD11	2.26	0.66
1:A:223:ALA:HA	1:A:247:VAL:HG21	1.77	0.66
3:C:34:ILE:CD1	3:C:120:VAL:HB	2.18	0.66
1:A:64:SER:HB3	1:A:219:SER:C	2.15	0.66
1:A:68:GLY:CA	1:A:218:PHE:CD1	2.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:HG11	1:A:526:LEU:HD21	1.76	0.66
1:A:529:ALA:HB2	1:A:551:LEU:CD1	2.24	0.66
1:A:369:ALA:HB2	1:A:463:ILE:HD11	1.77	0.66
1:A:282:LEU:HD23	1:A:331:GLN:HE21	1.61	0.66
1:A:378:MET:O	1:A:416:PRO:CD	2.43	0.66
1:A:559:SER:CB	1:A:560:PRO:HD3	2.25	0.66
3:C:163:LEU:HD21	3:C:204:THR:HG22	1.76	0.66
1:A:305:GLN:HB2	1:A:365:LEU:HD11	1.78	0.65
1:A:249:ASP:OD1	1:A:652:ARG:NH2	2.29	0.65
1:A:171:LEU:CD2	1:A:287:PHE:HE2	2.09	0.65
1:A:385:GLN:HB3	1:A:391:ARG:HD3	1.78	0.65
3:C:112:ILE:HG12	3:C:117:MET:HG3	1.76	0.65
1:A:68:GLY:HA2	1:A:218:PHE:CE1	2.31	0.65
2:B:85:LEU:CD1	2:B:422:LEU:HD11	2.27	0.65
1:A:162:ILE:HD12	1:A:164:TRP:CH2	2.33	0.64
1:A:397:LEU:HD21	1:A:439:VAL:HG23	1.78	0.64
1:A:162:ILE:HD11	1:A:164:TRP:CZ2	2.32	0.64
2:B:435:LEU:H	2:B:436:PRO:CD	2.09	0.64
1:A:68:GLY:CA	1:A:218:PHE:HE1	2.08	0.64
1:A:418:GLN:HE21	1:A:418:GLN:HA	1.63	0.64
1:A:434:ARG:O	1:A:435:ASN:HB2	1.95	0.64
1:A:95:MET:HE2	1:A:215:MET:CE	2.28	0.64
1:A:365:LEU:HD12	1:A:365:LEU:N	2.03	0.64
1:A:378:MET:HE3	1:A:398:LEU:CD2	2.27	0.64
1:A:579:VAL:HG12	1:A:620:CYS:O	1.98	0.64
2:B:249:ILE:O	2:B:253:ILE:HG22	1.97	0.64
3:C:112:ILE:H	3:C:112:ILE:CD1	2.10	0.64
1:A:223:ALA:CB	1:A:247:VAL:CG2	2.64	0.64
3:C:159:THR:HG21	3:C:210:TYR:CD1	2.33	0.64
3:C:112:ILE:CG1	3:C:117:MET:HG3	2.28	0.63
1:A:499:TYR:O	1:A:503:GLY:N	2.31	0.63
1:A:156:PHE:HD2	1:A:421:PRO:CB	2.05	0.63
1:A:185:ASP:OD1	1:A:187:ASN:N	2.29	0.63
1:A:260:LEU:HD21	1:A:312:LEU:CD2	2.27	0.63
1:A:559:SER:HB2	1:A:560:PRO:HD3	1.79	0.63
1:A:576:GLY:HA3	1:A:623:SER:HB3	1.81	0.63
1:A:622:ARG:HG2	1:A:622:ARG:NH1	2.04	0.63
1:A:260:LEU:HD12	1:A:313:GLN:HE22	1.63	0.62
1:A:524:GLY:HA2	1:A:531:ASN:HD21	1.64	0.62
1:A:95:MET:CG	1:A:120:GLY:O	2.47	0.62
1:A:268:THR:HG21	1:A:355:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ILE:HD11	2:B:238:ILE:HD13	1.81	0.62
1:A:500:GLU:O	1:A:503:GLY:HA2	1.98	0.62
1:A:378:MET:HE3	1:A:398:LEU:HD23	1.82	0.62
2:B:99:THR:HG21	2:B:181:TYR:CE1	2.34	0.62
1:A:268:THR:HG21	1:A:355:GLN:CD	2.21	0.62
3:C:61:ASP:O	3:C:62:ARG:HB2	1.98	0.62
1:A:249:ASP:OD1	1:A:652:ARG:NE	2.33	0.61
1:A:605:VAL:HG22	1:A:606:GLN:O	2.00	0.61
1:A:95:MET:SD	1:A:217:LEU:HD11	2.39	0.61
1:A:150:ASN:ND2	1:A:150:ASN:H	1.98	0.61
1:A:305:GLN:HB2	1:A:365:LEU:CD1	2.30	0.61
1:A:371:ARG:HH11	1:A:371:ARG:HB3	1.63	0.61
1:A:385:GLN:CA	1:A:391:ARG:HD3	2.30	0.61
1:A:152:TYR:CD1	1:A:383:VAL:HG21	2.27	0.61
1:A:422:LEU:CD2	1:A:423:PRO:HD2	2.22	0.61
1:A:511:VAL:O	1:A:511:VAL:HG13	2.01	0.61
2:B:85:LEU:HD13	2:B:422:LEU:HD11	1.82	0.61
2:B:424:LEU:O	2:B:428:PHE:HB2	2.00	0.61
1:A:337:TYR:HB3	1:A:429:ARG:HG3	1.83	0.60
2:B:207:VAL:CG1	4:D:26:LEU:HD21	2.31	0.60
1:A:54:LEU:HD23	1:A:59:GLN:HB2	1.82	0.60
1:A:155:GLU:CG	1:A:156:PHE:CE1	2.65	0.60
1:A:300:ALA:HB2	1:A:463:ILE:CD1	2.31	0.60
1:A:605:VAL:HG11	1:A:621:VAL:HG23	1.80	0.60
1:A:341:SER:CB	1:A:429:ARG:HH11	2.14	0.60
2:B:241:LEU:CD1	2:B:245:THR:HG21	2.31	0.60
1:A:260:LEU:CD1	1:A:313:GLN:NE2	2.64	0.60
1:A:371:ARG:HH11	1:A:371:ARG:CG	2.13	0.60
2:B:247:TRP:CE3	2:B:247:TRP:HA	2.36	0.60
1:A:66:ILE:HD13	1:A:220:HIS:CE1	2.36	0.60
1:A:96:VAL:CG2	1:A:121:LEU:HB3	2.32	0.60
1:A:304:THR:HG22	1:A:487:LEU:HG	1.83	0.60
1:A:98:LEU:HD13	1:A:107:LEU:HD21	1.84	0.60
1:A:133:GLY:HA2	1:A:452:TYR:CE1	2.35	0.60
1:A:260:LEU:HD12	1:A:313:GLN:NE2	2.17	0.60
2:B:435:LEU:HD12	2:B:439:ILE:CD1	2.32	0.60
4:D:45:PRO:HG2	4:D:46:ALA:H	1.66	0.60
2:B:244:TRP:CE3	2:B:247:TRP:CD1	2.76	0.60
1:A:51:VAL:HG22	1:A:221:MET:HE1	1.84	0.59
1:A:97:LEU:HD13	1:A:192:ILE:HG21	1.84	0.59
3:C:112:ILE:HD13	3:C:112:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HB	1:A:220:HIS:CE1	2.37	0.59
2:B:86:PHE:HZ	2:B:419:CYS:SG	2.21	0.59
3:C:159:THR:HG21	3:C:210:TYR:CE1	2.38	0.59
1:A:463:ILE:HG23	1:A:465:VAL:HG23	1.84	0.59
1:A:385:GLN:HB3	1:A:391:ARG:CD	2.32	0.59
1:A:162:ILE:CD1	1:A:164:TRP:CZ2	2.85	0.59
3:C:163:LEU:HD13	3:C:214:LEU:HD12	1.84	0.59
1:A:341:SER:HB2	1:A:429:ARG:HD2	1.85	0.58
1:A:101:LYS:CG	1:A:126:THR:HG21	2.33	0.58
1:A:279:ALA:HB1	1:A:328:VAL:HG13	1.85	0.58
1:A:313:GLN:HG2	1:A:575:THR:O	2.03	0.58
2:B:96:VAL:HG21	2:B:390:SER:CB	2.34	0.58
1:A:148:TYR:HE2	1:A:422:LEU:N	2.01	0.58
1:A:529:ALA:HB2	1:A:551:LEU:HD11	1.84	0.58
2:B:239:LYS:HG3	2:B:240:TYR:CD1	2.37	0.58
4:D:48:THR:OG1	4:D:49:GLU:HG2	2.03	0.58
1:A:250:PRO:HB3	1:A:635:PHE:HE2	1.66	0.58
4:D:51:SER:O	4:D:54:LYS:HG2	2.04	0.58
3:C:114:ILE:O	3:C:114:ILE:HD12	2.03	0.58
1:A:148:TYR:HE2	1:A:422:LEU:H	1.50	0.58
1:A:250:PRO:CB	1:A:635:PHE:CE2	2.83	0.57
1:A:295:ALA:O	1:A:300:ALA:N	2.34	0.57
1:A:434:ARG:HH11	1:A:434:ARG:CG	2.15	0.57
1:A:586:CYS:SG	1:A:604:TRP:HD1	2.26	0.57
1:A:559:SER:OG	1:A:560:PRO:HD3	2.04	0.57
1:A:96:VAL:CG2	1:A:118:ILE:HD11	2.31	0.57
1:A:123:VAL:HG23	1:A:123:VAL:O	2.03	0.57
1:A:430:PHE:HB3	1:A:436:ILE:HD11	1.87	0.57
3:C:30:LEU:O	3:C:34:ILE:HG23	2.04	0.57
4:D:40:GLU:O	4:D:44:VAL:CG2	2.41	0.57
3:C:34:ILE:CG1	3:C:120:VAL:CG1	2.83	0.57
1:A:186:GLU:OE1	1:A:189:THR:OG1	2.21	0.57
4:D:39:ARG:O	4:D:43:LEU:HB2	2.05	0.57
1:A:156:PHE:HD2	1:A:421:PRO:CD	2.18	0.56
1:A:304:THR:OG1	1:A:365:LEU:HD22	2.05	0.56
2:B:241:LEU:HG	2:B:245:THR:CG2	2.34	0.56
1:A:97:LEU:CD1	1:A:192:ILE:HG21	2.36	0.56
1:A:279:ALA:HB2	1:A:328:VAL:HG12	1.85	0.56
1:A:418:GLN:NE2	1:A:418:GLN:HA	2.20	0.56
2:B:244:TRP:CE3	2:B:244:TRP:HA	2.41	0.56
2:B:435:LEU:HD12	2:B:439:ILE:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:LEU:HD11	2:B:439:ILE:HD12	1.86	0.56
1:A:605:VAL:CG2	1:A:606:GLN:N	2.68	0.56
3:C:34:ILE:HD11	3:C:120:VAL:CG1	2.35	0.56
1:A:335:PHE:O	1:A:337:TYR:N	2.38	0.56
2:B:85:LEU:HD13	2:B:422:LEU:CD1	2.35	0.56
1:A:278:ALA:O	1:A:305:GLN:NE2	2.39	0.56
1:A:364:GLU:OE1	1:A:426:SER:N	2.38	0.56
1:A:156:PHE:CD2	1:A:421:PRO:CA	2.89	0.56
2:B:247:TRP:HA	2:B:247:TRP:HE3	1.71	0.56
1:A:222:HIS:O	1:A:651:SER:OG	2.23	0.55
1:A:296:GLU:OE1	1:A:450:ASN:HB2	2.05	0.55
1:A:95:MET:CE	1:A:217:LEU:HD21	2.36	0.55
1:A:101:LYS:HD3	1:A:126:THR:HG21	1.88	0.55
4:D:96:ILE:HG22	4:D:97:PRO:HD2	1.88	0.55
1:A:171:LEU:CG	1:A:287:PHE:HE2	2.19	0.55
1:A:339:GLY:HA2	1:A:630:ALA:HB1	1.87	0.55
1:A:516:GLN:O	1:A:519:THR:HG22	2.05	0.55
1:A:223:ALA:O	1:A:224:VAL:HG13	2.07	0.55
1:A:233:ARG:HB2	4:D:96:ILE:CD1	2.36	0.55
1:A:434:ARG:NH1	1:A:434:ARG:HG2	2.20	0.55
1:A:397:LEU:HD13	1:A:501:LEU:HD11	1.88	0.55
1:A:450:ASN:OD1	1:A:453:TYR:HA	2.07	0.55
1:A:633:PRO:CG	1:A:645:TYR:CD2	2.89	0.55
1:A:586:CYS:HG	1:A:604:TRP:HD1	1.54	0.55
3:C:34:ILE:HG13	3:C:120:VAL:CG1	2.37	0.55
1:A:54:LEU:CD2	1:A:59:GLN:HB2	2.37	0.55
1:A:299:VAL:HG11	1:A:526:LEU:CD2	2.37	0.55
2:B:241:LEU:CD1	2:B:245:THR:CG2	2.86	0.54
3:C:111:PRO:HG2	3:C:112:ILE:HD12	1.90	0.54
1:A:294:GLY:HA3	1:A:553:HIS:HD2	1.72	0.54
1:A:605:VAL:HG23	1:A:606:GLN:N	2.22	0.54
3:C:62:ARG:HG2	3:C:68:GLN:OE1	2.07	0.54
1:A:385:GLN:O	1:A:391:ARG:HB2	2.07	0.54
1:A:540:GLN:HG2	1:A:606:GLN:HE22	1.67	0.54
2:B:408:ILE:HD13	3:C:131:VAL:HG11	1.90	0.54
1:A:224:VAL:HG21	4:D:100:THR:C	2.28	0.54
1:A:347:MET:SD	1:A:352:PHE:CE2	3.01	0.54
1:A:260:LEU:CD1	1:A:313:GLN:HE22	2.20	0.54
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.13	0.54
1:A:369:ALA:HB1	1:A:463:ILE:CG1	2.38	0.54
1:A:422:LEU:HD22	1:A:423:PRO:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:OH	1:A:428:GLN:NE2	2.41	0.54
1:A:559:SER:CB	1:A:560:PRO:CD	2.86	0.53
3:C:90:TYR:HE2	3:C:121:SER:HB2	1.74	0.53
1:A:156:PHE:HD2	1:A:421:PRO:HD3	1.72	0.53
1:A:552:GLN:OE1	1:A:552:GLN:HA	2.09	0.53
1:A:529:ALA:CB	1:A:551:LEU:HD11	2.38	0.53
3:C:40:PHE:O	3:C:44:VAL:HG23	2.09	0.53
1:A:506:ASN:O	1:A:507:PHE:HD1	1.91	0.53
1:A:222:HIS:O	1:A:223:ALA:HB3	2.09	0.53
4:D:31:LEU:HD13	4:D:64:PHE:CZ	2.43	0.53
1:A:289:TRP:NE1	1:A:650:GLU:OE2	2.40	0.53
1:A:341:SER:HB2	1:A:429:ARG:HH11	1.73	0.53
1:A:152:TYR:CE1	1:A:383:VAL:CB	2.91	0.53
1:A:385:GLN:CB	1:A:391:ARG:HD3	2.39	0.53
2:B:241:LEU:HD11	2:B:245:THR:HG21	1.91	0.53
1:A:200:ASN:HD21	1:A:213:CYS:HB3	1.74	0.53
5:H:1:NAG:O3	5:H:2:NAG:H83	2.09	0.53
1:A:288:PHE:CE2	1:A:456:ILE:HD11	2.44	0.53
1:A:633:PRO:CG	1:A:645:TYR:HD2	2.20	0.53
1:A:443:ASP:OD1	1:A:444:HIS:ND1	2.41	0.52
1:A:164:TRP:CZ2	1:A:423:PRO:HA	2.43	0.52
2:B:242:PRO:HD2	2:B:245:THR:HB	1.90	0.52
1:A:40:ILE:HD11	3:C:157:PHE:HZ	1.74	0.52
1:A:369:ALA:CB	1:A:463:ILE:HD11	2.39	0.52
1:A:268:THR:CG2	1:A:355:GLN:CG	2.60	0.52
3:C:34:ILE:HG12	3:C:120:VAL:HG11	1.91	0.52
1:A:82:LEU:HD23	1:A:110:LYS:NZ	2.25	0.52
3:C:34:ILE:HB	3:C:90:TYR:OH	2.09	0.52
1:A:68:GLY:HA2	1:A:218:PHE:HD1	1.74	0.52
3:C:126:GLY:O	3:C:168:ILE:HG12	2.09	0.52
3:C:137:ILE:HD11	3:C:160:SER:OG	2.10	0.52
1:A:104:THR:HG22	1:A:105:ARG:H	1.75	0.52
1:A:645:TYR:O	1:A:646:SER:OG	2.23	0.52
1:A:155:GLU:CG	1:A:156:PHE:CD1	2.89	0.52
1:A:162:ILE:CG2	1:A:420:GLN:OE1	2.55	0.52
1:A:182:LEU:HD13	1:A:288:PHE:CE2	2.44	0.52
2:B:241:LEU:CG	2:B:245:THR:HG22	2.38	0.52
1:A:91:ASN:O	1:A:93:PRO:HD2	2.10	0.51
1:A:40:ILE:HD11	3:C:157:PHE:CZ	2.45	0.51
1:A:64:SER:HB3	1:A:219:SER:N	2.23	0.51
1:A:66:ILE:HB	1:A:220:HIS:NE2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:O	1:A:163:GLN:HB2	2.08	0.51
1:A:326:MET:HG3	1:A:326:MET:O	2.09	0.51
2:B:106:TYR:CG	2:B:235:LEU:HD22	2.45	0.51
3:C:106:GLU:OE1	3:C:106:GLU:HA	2.10	0.51
4:D:97:PRO:HG2	4:D:100:THR:OG1	2.11	0.51
1:A:269:LEU:HD13	1:A:358:ASN:HD22	1.76	0.51
1:A:443:ASP:OD1	1:A:444:HIS:N	2.43	0.51
1:A:605:VAL:HG11	1:A:621:VAL:HG21	1.92	0.51
2:B:435:LEU:CD1	2:B:439:ILE:HD12	2.41	0.51
1:A:249:ASP:OD1	1:A:652:ARG:CZ	2.59	0.51
1:A:562:ASN:OD1	1:A:562:ASN:N	2.43	0.51
1:A:224:VAL:CG1	4:D:99:GLY:O	2.58	0.51
1:A:372:THR:CG2	1:A:449:HIS:CD2	2.93	0.51
3:C:90:TYR:CE2	3:C:94:LEU:CD1	2.87	0.51
3:C:170:LEU:HG	3:C:174:TRP:CZ2	2.46	0.51
4:D:44:VAL:CG1	4:D:47:TYR:CD1	2.86	0.51
1:A:280:THR:CG2	1:A:365:LEU:HD13	2.41	0.51
1:A:390:VAL:CG2	7:A:1705:NAG:H82	2.41	0.51
2:B:250:LEU:O	2:B:439:ILE:HG21	2.10	0.51
1:A:60:ILE:HG12	1:A:648:TRP:CZ3	2.46	0.51
1:A:343:MET:CE	1:A:347:MET:SD	2.98	0.51
1:A:559:SER:HB2	1:A:560:PRO:CD	2.40	0.51
1:A:102:HIS:O	1:A:107:LEU:HD23	2.11	0.50
1:A:283:ASP:HA	1:A:553:HIS:HB3	1.93	0.50
1:A:425:SER:O	1:A:428:GLN:N	2.44	0.50
1:A:635:PHE:CZ	1:A:649:THR:CG2	2.93	0.50
1:A:693:LYS:NZ	3:C:242:SER:O	2.44	0.50
1:A:364:GLU:O	1:A:440:VAL:HA	2.11	0.50
2:B:402:GLY:O	2:B:404:TRP:N	2.44	0.50
2:B:448:ALA:CB	3:C:47:LEU:HD21	2.40	0.50
1:A:95:MET:SD	1:A:215:MET:HE2	2.52	0.50
1:A:633:PRO:CB	1:A:645:TYR:CE2	2.89	0.50
2:B:82:VAL:HB	3:C:33:ILE:HD11	1.93	0.50
2:B:416:ILE:CD1	3:C:40:PHE:HB2	2.42	0.50
1:A:540:GLN:CG	1:A:606:GLN:NE2	2.39	0.50
1:A:633:PRO:HD2	1:A:645:TYR:CD2	2.47	0.50
2:B:240:TYR:CD1	2:B:240:TYR:N	2.77	0.50
1:A:145:PHE:CG	1:A:336:ASP:HB3	2.47	0.50
1:A:506:ASN:C	1:A:507:PHE:CD1	2.85	0.50
2:B:435:LEU:HD11	2:B:439:ILE:HD11	1.89	0.50
1:A:162:ILE:CD1	1:A:164:TRP:CH2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HG	1:A:287:PHE:HE2	1.75	0.50
1:A:270:LYS:HG3	1:A:271:PRO:CD	2.42	0.50
1:A:631:LEU:HD23	1:A:635:PHE:HB2	1.94	0.50
2:B:253:ILE:HD13	2:B:388:PHE:CZ	2.46	0.50
1:A:622:ARG:NH1	1:A:622:ARG:CG	2.73	0.50
1:A:58:HIS:ND1	1:A:58:HIS:N	2.60	0.49
1:A:152:TYR:CZ	1:A:383:VAL:CG1	2.89	0.49
1:A:633:PRO:CD	1:A:645:TYR:HD2	2.25	0.49
1:A:223:ALA:N	1:A:247:VAL:HG21	2.25	0.49
1:A:250:PRO:HB3	1:A:635:PHE:HD2	1.64	0.49
1:A:557:VAL:HG13	1:A:558:SER:N	2.26	0.49
1:A:68:GLY:H	1:A:218:PHE:HD1	1.55	0.49
1:A:230:CYS:SG	1:A:247:VAL:CG1	2.91	0.49
1:A:280:THR:HG23	1:A:365:LEU:HD13	1.93	0.49
2:B:244:TRP:O	2:B:248:LEU:N	2.34	0.49
4:D:96:ILE:CG2	4:D:97:PRO:HD2	2.42	0.49
1:A:49:PRO:HD3	1:A:656:ILE:HD13	1.93	0.49
1:A:605:VAL:CG2	1:A:606:GLN:O	2.61	0.49
2:B:466:TYR:CZ	3:C:163:LEU:HD23	2.47	0.49
3:C:24:THR:HG21	3:C:119:TYR:CE1	2.47	0.49
3:C:42:TRP:CH2	3:C:46:LEU:HD12	2.47	0.49
1:A:152:TYR:CE1	1:A:383:VAL:HG11	2.47	0.49
1:A:152:TYR:CD1	1:A:152:TYR:C	2.86	0.49
1:A:418:GLN:CA	1:A:418:GLN:NE2	2.73	0.49
3:C:10:THR:CB	3:C:138:LEU:HD21	2.43	0.49
3:C:80:VAL:HG11	3:C:198:LEU:HD12	1.94	0.49
3:C:122:GLY:HA3	3:C:172:THR:HA	1.94	0.49
1:A:82:LEU:HD23	1:A:110:LYS:HZ2	1.78	0.49
1:A:385:GLN:HA	1:A:391:ARG:HB2	1.93	0.49
3:C:227:TRP:O	3:C:231:THR:HG23	2.13	0.49
1:A:74:HIS:N	1:A:95:MET:O	2.45	0.49
1:A:152:TYR:O	1:A:154:PRO:CD	2.47	0.49
1:A:222:HIS:N	1:A:222:HIS:CD2	2.78	0.49
1:A:274:ARG:HD2	1:A:360:ASP:OD2	2.13	0.49
2:B:211:ILE:O	2:B:215:TRP:N	2.45	0.49
1:A:72:VAL:HG13	1:A:94:TYR:CE1	2.48	0.49
1:A:222:HIS:HB3	1:A:247:VAL:HG23	1.95	0.49
1:A:378:MET:SD	1:A:413:LEU:CD2	3.01	0.48
2:B:385:ASP:OD1	2:B:435:LEU:HD22	2.12	0.48
1:A:121:LEU:O	1:A:180:ILE:HA	2.13	0.48
1:A:224:VAL:O	1:A:225:ILE:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:LEU:HD13	2:B:392:LEU:HD12	1.93	0.48
1:A:57:THR:HG22	1:A:58:HIS:ND1	2.28	0.48
1:A:101:LYS:CD	1:A:126:THR:HG21	2.42	0.48
1:A:152:TYR:OH	1:A:383:VAL:HB	2.13	0.48
1:A:365:LEU:H	1:A:365:LEU:CD1	2.08	0.48
1:A:629:ARG:CZ	1:A:631:LEU:HD12	2.43	0.48
3:C:80:VAL:CG1	3:C:198:LEU:HD12	2.43	0.48
3:C:115:ARG:CB	3:C:115:ARG:HH11	2.27	0.48
2:B:182:LEU:HD22	2:B:202:ILE:CD1	2.44	0.48
2:B:239:LYS:CG	2:B:240:TYR:CD1	2.93	0.48
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.13	0.48
1:A:311:ALA:CA	1:A:511:VAL:HG23	2.44	0.48
2:B:387:ILE:O	2:B:391:VAL:HG23	2.13	0.48
1:A:290:ASN:O	1:A:552:GLN:CG	2.59	0.48
1:A:419:SER:O	1:A:419:SER:OG	2.30	0.47
1:A:609:LEU:CD2	1:A:614:THR:HA	2.44	0.47
2:B:91:LEU:O	2:B:95:VAL:HG23	2.14	0.47
3:C:62:ARG:CG	3:C:68:GLN:OE1	2.61	0.47
3:C:206:LEU:HD23	3:C:212:ALA:HB1	1.95	0.47
1:A:269:LEU:CD1	1:A:358:ASN:HD22	2.27	0.47
1:A:294:GLY:O	1:A:299:VAL:HG23	2.14	0.47
1:A:341:SER:OG	1:A:429:ARG:NH1	2.47	0.47
1:A:679:ILE:HG21	3:C:12:VAL:HA	1.96	0.47
1:A:385:GLN:O	1:A:391:ARG:HD3	2.14	0.47
1:A:451:LYS:HB2	1:A:451:LYS:HZ3	1.76	0.47
3:C:61:ASP:O	3:C:62:ARG:CB	2.63	0.47
4:D:39:ARG:O	4:D:43:LEU:CB	2.62	0.47
1:A:122:ALA:HA	1:A:181:PHE:O	2.15	0.47
1:A:432:ARG:HH12	1:A:644:GLU:CB	2.09	0.47
1:A:60:ILE:HG22	1:A:173:TYR:O	2.15	0.47
1:A:371:ARG:HD3	1:A:376:LEU:CD1	2.45	0.47
4:D:47:TYR:CB	4:D:50:GLN:CB	2.63	0.47
1:A:349:LYS:HB3	1:A:351:LYS:HD2	1.97	0.47
1:A:369:ALA:CB	1:A:463:ILE:CG1	2.92	0.47
1:A:552:GLN:HG2	5:J:1:NAG:C8	2.45	0.47
1:A:66:ILE:CD1	1:A:220:HIS:ND1	2.76	0.47
1:A:98:LEU:CD1	1:A:107:LEU:HD21	2.45	0.47
1:A:369:ALA:CB	1:A:463:ILE:HG13	2.45	0.47
1:A:427:LEU:HD12	1:A:427:LEU:O	2.15	0.47
2:B:208:VAL:HG21	4:D:28:PHE:CD1	2.50	0.47
2:B:208:VAL:O	2:B:211:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:PRO:HD2	1:A:645:TYR:HD2	1.80	0.47
2:B:211:ILE:HD12	2:B:212:SER:N	2.30	0.47
3:C:112:ILE:CD1	3:C:112:ILE:N	2.73	0.47
1:A:68:GLY:HA3	1:A:218:PHE:HE1	1.81	0.46
1:A:304:THR:OG1	1:A:365:LEU:CD2	2.63	0.46
1:A:164:TRP:HB3	1:A:448:PHE:CE1	2.50	0.46
1:A:269:LEU:HA	1:A:269:LEU:HD23	1.79	0.46
3:C:90:TYR:CE2	3:C:121:SER:HB2	2.50	0.46
3:C:174:TRP:CZ2	3:C:197:HIS:HA	2.50	0.46
1:A:76:VAL:HB	1:A:98:LEU:HD23	1.98	0.46
1:A:503:GLY:O	1:A:505:THR:HG23	2.15	0.46
1:A:253:ASP:O	1:A:630:ALA:HB3	2.16	0.46
1:A:377:TRP:CE3	1:A:415:ARG:O	2.69	0.46
2:B:80:LYS:O	2:B:83:ILE:HG22	2.15	0.46
1:A:343:MET:HE2	1:A:347:MET:SD	2.56	0.46
1:A:53:LEU:HD21	1:A:554:TYR:OH	2.16	0.46
1:A:63:GLN:HG3	1:A:221:MET:HB2	1.98	0.46
2:B:207:VAL:HG11	4:D:26:LEU:HD21	1.97	0.46
4:D:3:LEU:O	4:D:11:LYS:HE2	2.16	0.46
1:A:152:TYR:OH	1:A:383:VAL:CG1	2.64	0.46
1:A:281:ARG:HD3	1:A:297:SER:O	2.15	0.46
4:D:97:PRO:HB2	4:D:100:THR:OG1	2.15	0.46
1:A:233:ARG:HB2	4:D:96:ILE:HD13	1.97	0.45
2:B:241:LEU:HD11	2:B:245:THR:CG2	2.46	0.45
4:D:44:VAL:HG11	4:D:47:TYR:HD1	1.66	0.45
1:A:268:THR:HA	1:A:353:PRO:HA	1.97	0.45
1:A:285:ARG:HG2	1:A:334:THR:OG1	2.16	0.45
1:A:306:LEU:HD23	1:A:306:LEU:O	2.17	0.45
2:B:234:ALA:HA	2:B:391:VAL:HG22	1.98	0.45
1:A:300:ALA:CB	1:A:369:ALA:HB2	2.44	0.45
1:A:253:ASP:OD1	1:A:555:ILE:HG23	2.17	0.45
1:A:253:ASP:CB	1:A:559:SER:O	2.61	0.45
1:A:275:VAL:HG12	1:A:324:ASN:HB3	1.98	0.45
1:A:644:GLU:HG2	1:A:645:TYR:HD1	1.80	0.45
1:A:397:LEU:HD21	1:A:439:VAL:CG2	2.42	0.45
1:A:128:PRO:O	1:A:129:SER:CB	2.56	0.45
1:A:279:ALA:CA	1:A:328:VAL:HG13	2.46	0.45
1:A:367:GLN:HE21	1:A:367:GLN:HB3	1.58	0.45
3:C:106:GLU:O	3:C:107:ASP:HB2	2.15	0.45
4:D:31:LEU:HD13	4:D:64:PHE:CE2	2.52	0.45
1:A:95:MET:HE1	1:A:217:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ALA:HB1	1:A:230:CYS:SG	2.57	0.45
1:A:583:ARG:HB2	1:A:604:TRP:CZ2	2.51	0.45
3:C:34:ILE:HG13	3:C:120:VAL:HG12	1.98	0.45
1:A:157:ALA:O	1:A:158:HIS:ND1	2.50	0.45
1:A:164:TRP:CZ2	1:A:423:PRO:CA	3.00	0.45
1:A:95:MET:HE1	1:A:215:MET:CE	2.47	0.45
1:A:96:VAL:O	1:A:121:LEU:HB2	2.17	0.45
1:A:280:THR:OG1	1:A:305:GLN:CB	2.64	0.45
1:A:341:SER:HB2	1:A:429:ARG:NH1	2.32	0.45
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.83	0.45
1:A:57:THR:CG2	1:A:58:HIS:CE1	3.00	0.44
1:A:283:ASP:OD2	1:A:555:ILE:HD11	2.17	0.44
4:D:44:VAL:HG12	4:D:46:ALA:O	2.17	0.44
1:A:634:ALA:HB2	1:A:645:TYR:HB2	2.00	0.44
1:A:637:LEU:CB	1:A:639:GLN:HG2	2.47	0.44
1:A:156:PHE:CD2	1:A:421:PRO:HD3	2.52	0.44
1:A:311:ALA:CB	1:A:511:VAL:CG2	2.95	0.44
2:B:83:ILE:HG21	3:C:29:PRO:HB3	1.99	0.44
3:C:34:ILE:HG13	3:C:35:LEU:N	2.32	0.44
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.73	0.44
1:A:397:LEU:CG	1:A:439:VAL:HG21	2.43	0.44
1:A:498:LEU:O	1:A:502:ALA:N	2.32	0.44
2:B:92:CYS:O	2:B:96:VAL:HG23	2.17	0.44
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.81	0.44
3:C:12:VAL:O	3:C:165:ALA:HB2	2.18	0.44
1:A:95:MET:CE	1:A:215:MET:HE3	2.39	0.44
1:A:377:TRP:HA	1:A:414:ARG:O	2.17	0.44
2:B:416:ILE:CD1	3:C:36:VAL:HG12	2.48	0.44
1:A:264:ASN:O	1:A:265:THR:CB	2.66	0.44
1:A:586:CYS:HB2	1:A:620:CYS:SG	2.46	0.44
2:B:85:LEU:HD21	2:B:381:LEU:HD23	1.98	0.44
1:A:182:LEU:HD23	1:A:184:GLU:HG3	1.99	0.44
1:A:425:SER:O	1:A:426:SER:C	2.56	0.44
3:C:42:TRP:CZ3	3:C:46:LEU:HD12	2.52	0.44
1:A:139:GLN:HG2	1:A:163:GLN:CG	2.35	0.44
1:A:284:SER:OG	1:A:553:HIS:HB2	2.17	0.44
1:A:68:GLY:N	1:A:218:PHE:HD1	2.11	0.44
1:A:95:MET:HG3	1:A:120:GLY:O	2.17	0.43
1:A:632:SER:HB3	1:A:645:TYR:O	2.17	0.43
2:B:250:LEU:CD1	2:B:392:LEU:HG	2.48	0.43
1:A:185:ASP:HB3	1:A:188:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:O	1:A:302:PHE:CD2	2.71	0.43
3:C:90:TYR:HE2	3:C:94:LEU:HD11	1.72	0.43
4:D:97:PRO:HG2	4:D:100:THR:HG1	1.83	0.43
1:A:103:PHE:O	1:A:103:PHE:CG	2.70	0.43
1:A:337:TYR:CB	1:A:429:ARG:HG3	2.47	0.43
1:A:441:LEU:HD12	1:A:494:LEU:HD12	2.00	0.43
2:B:416:ILE:HD11	3:C:36:VAL:HG12	1.98	0.43
3:C:7:PHE:O	3:C:10:THR:HG22	2.19	0.43
3:C:80:VAL:HG13	3:C:197:HIS:CG	2.54	0.43
4:D:34:ILE:CD1	4:D:61:ALA:HA	2.48	0.43
1:A:192:ILE:HG12	1:A:660:ILE:HD12	2.01	0.43
1:A:102:HIS:O	1:A:104:THR:N	2.50	0.43
1:A:366:GLY:O	1:A:442:ALA:HA	2.18	0.43
1:A:534:PHE:CE2	1:A:566:VAL:HG11	2.53	0.43
2:B:100:ILE:CD1	2:B:238:ILE:HD13	2.48	0.43
2:B:241:LEU:HD21	2:B:249:ILE:HD12	2.00	0.43
1:A:156:PHE:CD2	1:A:421:PRO:CD	2.99	0.43
1:A:390:VAL:HG23	7:A:1705:NAG:H82	2.00	0.43
3:C:62:ARG:HG2	3:C:68:GLN:CD	2.38	0.43
3:C:31:ARG:O	3:C:34:ILE:HG12	2.19	0.43
4:D:26:LEU:HB3	4:D:29:LEU:HB2	2.00	0.43
1:A:68:GLY:N	1:A:218:PHE:HE1	2.12	0.43
1:A:311:ALA:HB1	1:A:511:VAL:HG23	1.98	0.43
1:A:662:LEU:HD13	3:C:149:ILE:HA	2.01	0.43
1:A:224:VAL:CG2	4:D:100:THR:O	2.57	0.43
1:A:367:GLN:O	1:A:443:ASP:CG	2.56	0.43
2:B:452:LEU:HD13	3:C:51:VAL:CG2	2.48	0.43
3:C:91:TYR:CE1	3:C:182:CYS:SG	3.11	0.43
1:A:279:ALA:O	1:A:364:GLU:HA	2.18	0.43
1:A:299:VAL:CG2	1:A:553:HIS:CD2	3.02	0.43
2:B:432:LEU:N	2:B:433:PRO:HD3	2.34	0.43
1:A:97:LEU:HD13	1:A:192:ILE:CG2	2.49	0.42
1:A:112:LYS:HB3	1:A:112:LYS:HE2	1.82	0.42
3:C:112:ILE:HG13	3:C:117:MET:HG3	2.01	0.42
1:A:583:ARG:HA	1:A:604:TRP:NE1	2.35	0.42
1:A:605:VAL:HG13	1:A:619:ARG:O	2.19	0.42
1:A:306:LEU:HG	1:A:329:PHE:CE2	2.55	0.42
1:A:334:THR:HG23	1:A:335:PHE:CD2	2.55	0.42
1:A:385:GLN:C	1:A:391:ARG:HD3	2.40	0.42
1:A:157:ALA:C	1:A:158:HIS:ND1	2.73	0.42
1:A:341:SER:CB	1:A:429:ARG:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HA	1:A:356:LEU:HD12	1.75	0.42
1:A:396:ASP:O	1:A:400:THR:HG23	2.19	0.42
2:B:465:PHE:HA	3:C:204:THR:HB	2.01	0.42
3:C:60:THR:HG21	3:C:67:LEU:CD2	2.45	0.42
1:A:312:LEU:HD11	1:A:498:LEU:CB	2.50	0.42
1:A:552:GLN:HG2	5:J:1:NAG:H81	2.00	0.42
2:B:174:LEU:HD22	2:B:206:GLY:HA2	2.00	0.42
3:C:243:LEU:O	3:C:243:LEU:HD22	2.18	0.42
1:A:296:GLU:OE1	1:A:367:GLN:NE2	2.48	0.42
1:A:54:LEU:CD1	1:A:248:CYS:SG	3.06	0.42
1:A:74:HIS:O	1:A:96:VAL:HA	2.18	0.42
1:A:378:MET:HE1	1:A:415:ARG:HE	1.84	0.42
1:A:296:GLU:HG3	1:A:370:LEU:HD21	2.01	0.42
1:A:345:TYR:CE2	1:A:349:LYS:HE2	2.55	0.42
2:B:244:TRP:CE3	2:B:244:TRP:CA	3.03	0.42
3:C:17:ALA:CB	3:C:168:ILE:HG21	2.41	0.42
3:C:60:THR:O	3:C:61:ASP:HB3	2.20	0.42
2:B:186:PHE:CD1	2:B:193:VAL:HG21	2.55	0.42
4:D:38:PHE:CD1	4:D:38:PHE:C	2.92	0.42
1:A:279:ALA:HA	1:A:328:VAL:HG13	2.02	0.41
2:B:235:LEU:HD23	2:B:235:LEU:HA	1.91	0.41
2:B:247:TRP:CH2	2:B:395:LYS:HB3	2.53	0.41
3:C:34:ILE:CD1	3:C:120:VAL:CG1	2.98	0.41
3:C:163:LEU:HD21	3:C:204:THR:CG2	2.47	0.41
4:D:34:ILE:HD11	4:D:61:ALA:HA	2.01	0.41
4:D:45:PRO:HG2	4:D:46:ALA:N	2.34	0.41
1:A:234:SER:OG	1:A:246:ILE:HG23	2.19	0.41
2:B:195:TYR:CZ	4:D:94:PHE:HB2	2.55	0.41
1:A:158:HIS:O	1:A:159:CYS:SG	2.79	0.41
1:A:162:ILE:HD11	1:A:421:PRO:HG2	2.03	0.41
1:A:185:ASP:OD1	1:A:186:GLU:N	2.53	0.41
1:A:222:HIS:CB	1:A:247:VAL:HG23	2.50	0.41
1:A:279:ALA:HB1	1:A:330:PHE:CD2	2.53	0.41
1:A:429:ARG:NH2	1:A:432:ARG:NH1	2.68	0.41
2:B:433:PRO:HB3	2:B:436:PRO:HG3	2.02	0.41
1:A:162:ILE:HD12	1:A:164:TRP:CZ2	2.54	0.41
1:A:672:THR:HG23	3:C:158:LEU:HD13	2.03	0.41
2:B:193:VAL:HG12	2:B:198:VAL:HG23	2.02	0.41
1:A:68:GLY:CA	1:A:218:PHE:HD1	2.30	0.41
1:A:453:TYR:CD2	1:A:454:GLN:HG2	2.55	0.41
1:A:553:HIS:HD1	1:A:563:THR:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ARG:NH1	8:C:1245:PC1:O12	2.48	0.41
1:A:258:SER:HB2	1:A:571:LEU:HD21	2.03	0.41
1:A:375:GLU:HA	1:A:412:ILE:HG23	2.02	0.41
1:A:451:LYS:NZ	1:A:451:LYS:CB	2.73	0.41
1:A:159:CYS:SG	1:A:159:CYS:O	2.79	0.41
2:B:251:ALA:O	2:B:255:VAL:HG23	2.21	0.41
3:C:91:TYR:CZ	3:C:182:CYS:SG	3.13	0.41
4:D:82:ARG:NH2	4:D:97:PRO:HG3	2.35	0.41
1:A:57:THR:CG2	1:A:58:HIS:ND1	2.83	0.41
1:A:234:SER:HB2	1:A:247:VAL:HG12	2.02	0.41
1:A:352:PHE:CD1	1:A:353:PRO:HD2	2.56	0.41
1:A:672:THR:HG23	3:C:158:LEU:CD1	2.50	0.41
2:B:246:ALA:HB1	2:B:395:LYS:HG3	2.02	0.41
1:A:64:SER:HB3	1:A:219:SER:O	2.20	0.41
1:A:101:LYS:HG2	1:A:126:THR:HG21	2.02	0.41
1:A:167:LEU:HD22	1:A:451:LYS:HG2	2.02	0.41
1:A:215:MET:HE2	1:A:215:MET:HB3	1.79	0.41
1:A:304:THR:HG22	1:A:487:LEU:CG	2.51	0.41
1:A:361:SER:CB	1:A:501:LEU:HD13	2.48	0.41
1:A:52:ARG:HG2	1:A:54:LEU:HD21	2.03	0.40
1:A:256:VAL:HG21	1:A:567:VAL:CG1	2.48	0.40
1:A:349:LYS:HB3	1:A:351:LYS:CD	2.50	0.40
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.85	0.40
1:A:140:CYS:CB	1:A:159:CYS:HG	2.33	0.40
2:B:241:LEU:HD12	2:B:241:LEU:HA	1.76	0.40
1:A:328:VAL:HG22	1:A:329:PHE:N	2.36	0.40
1:A:460:ALA:HB1	1:A:465:VAL:HB	2.03	0.40
2:B:192:ALA:HB3	4:D:79:GLN:HE22	1.86	0.40
2:B:248:LEU:HD22	2:B:252:VAL:HG23	2.03	0.40
1:A:53:LEU:HB2	1:A:60:ILE:HD11	2.02	0.40
1:A:60:ILE:HG12	1:A:648:TRP:HZ3	1.85	0.40
1:A:169:ASN:HD22	1:A:171:LEU:HB2	1.85	0.40
1:A:332:GLY:HA2	1:A:555:ILE:HG12	2.03	0.40
1:A:378:MET:HA	1:A:440:VAL:O	2.21	0.40
3:C:35:LEU:HA	3:C:124:SER:HB2	2.03	0.40
1:A:60:ILE:O	1:A:60:ILE:HG13	2.22	0.40
1:A:283:ASP:CG	1:A:555:ILE:HD11	2.42	0.40
1:A:380:THR:O	1:A:382:PRO:HD3	2.21	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	663/709 (94%)	589 (89%)	54 (8%)	20 (3%)	4 23
2	B	209/467 (45%)	196 (94%)	8 (4%)	5 (2%)	6 28
3	C	241/265 (91%)	228 (95%)	12 (5%)	1 (0%)	34 67
4	D	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
All	All	1211/1542 (78%)	1108 (92%)	77 (6%)	26 (2%)	10 30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	SER
1	A	559	SER
1	A	210	PHE
1	A	333	GLU
1	A	371	ARG
1	A	435	ASN
1	A	454	GLN
1	A	473	PRO
2	B	216	LYS
2	B	403	ASP
1	A	211	PRO
1	A	612	ASN
2	B	105	PHE
1	A	88	ASP
1	A	560	PRO
1	A	163	GLN
1	A	223	ALA
1	A	353	PRO
2	B	435	LEU
3	C	107	ASP
1	A	89	GLY
1	A	646	SER

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Mol	Chain	Res	Type
1	A	655	ASP
1	A	480	VAL
2	B	432	LEU
1	A	129	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	583/612 (95%)	497 (85%)	86 (15%)	3 12
2	B	184/408 (45%)	165 (90%)	19 (10%)	7 26
3	C	193/214 (90%)	171 (89%)	22 (11%)	5 21
4	D	88/89 (99%)	77 (88%)	11 (12%)	4 17
All	All	1048/1323 (79%)	910 (87%)	138 (13%)	7 15

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	59	GLN
1	A	60	ILE
1	A	69	ASP
1	A	84	TRP
1	A	85	VAL
1	A	86	LEU
1	A	94	TYR
1	A	95	MET
1	A	97	LEU
1	A	101	LYS
1	A	104	THR
1	A	107	LEU
1	A	111	LEU
1	A	112	LYS
1	A	121	LEU
1	A	126	THR

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Mol	Chain	Res	Type
1	A	129	SER
1	A	132	SER
1	A	139	GLN
1	A	147	VAL
1	A	149	SER
1	A	150	ASN
1	A	152	TYR
1	A	155	GLU
1	A	162	ILE
1	A	163	GLN
1	A	174	GLU
1	A	182	LEU
1	A	201	LEU
1	A	210	PHE
1	A	217	LEU
1	A	248	CYS
1	A	249	ASP
1	A	264	ASN
1	A	270	LYS
1	A	273	ASP
1	A	280	THR
1	A	281	ARG
1	A	296	GLU
1	A	302	PHE
1	A	305	GLN
1	A	306	LEU
1	A	312	LEU
1	A	326	MET
1	A	333	GLU
1	A	342	ARG
1	A	343	MET
1	A	347	MET
1	A	349	LYS
1	A	364	GLU
1	A	365	LEU
1	A	367	GLN
1	A	371	ARG
1	A	378	MET
1	A	380	THR
1	A	387	ASN
1	A	391	ARG
1	A	413	LEU

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Mol	Chain	Res	Type
1	A	418	GLN
1	A	425	SER
1	A	429	ARG
1	A	431	LEU
1	A	434	ARG
1	A	436	ILE
1	A	437	SER
1	A	463	ILE
1	A	464	ASN
1	A	487	LEU
1	A	537	ILE
1	A	561	THR
1	A	562	ASN
1	A	574	LEU
1	A	586	CYS
1	A	604	TRP
1	A	605	VAL
1	A	609	LEU
1	A	624	THR
1	A	631	LEU
1	A	632	SER
1	A	636	GLU
1	A	637	LEU
1	A	638	SER
1	A	643	THR
1	A	644	GLU
1	A	695	ASP
2	B	84	MET
2	B	85	LEU
2	B	91	LEU
2	B	174	LEU
2	B	180	ILE
2	B	241	LEU
2	B	244	TRP
2	B	248	LEU
2	B	381	LEU
2	B	395	LYS
2	B	407	THR
2	B	420	LEU
2	B	422	LEU
2	B	423	LEU
2	B	424	LEU

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Mol	Chain	Res	Type
2	B	425	LEU
2	B	427	ILE
2	B	429	LYS
2	B	435	LEU
3	C	46	LEU
3	C	47	LEU
3	C	64	ASP
3	C	68	GLN
3	C	91	TYR
3	C	93	LEU
3	C	106	GLU
3	C	112	ILE
3	C	113	SER
3	C	114	ILE
3	C	123	LEU
3	C	127	ILE
3	C	133	SER
3	C	146	VAL
3	C	170	LEU
3	C	192	LEU
3	C	206	LEU
3	C	207	ASN
3	C	218	TYR
3	C	242	SER
3	C	243	LEU
3	C	244	LEU
4	D	14	LEU
4	D	38	PHE
4	D	39	ARG
4	D	40	GLU
4	D	42	PHE
4	D	43	LEU
4	D	47	TYR
4	D	50	GLN
4	D	67	TRP
4	D	94	PHE
4	D	98	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	150	ASN
1	A	163	GLN
1	A	169	ASN
1	A	222	HIS
1	A	305	GLN
1	A	313	GLN
1	A	331	GLN
1	A	358	ASN
1	A	393	GLN
1	A	418	GLN
1	A	428	GLN
1	A	478	ASN
1	A	516	GLN
1	A	531	ASN
1	A	606	GLN
1	A	639	GLN
3	C	116	GLN
3	C	136	ASN
3	C	207	ASN
4	D	8	ASN
4	D	79	GLN

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)

15 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	1,5	14,14,15	0.58	0	17,19,21	1.07	1 (5%)
5	NAG	E	2	5	14,14,15	0.52	0	17,19,21	1.29	2 (11%)
6	NAG	F	1	1,6	14,14,15	0.49	0	17,19,21	1.50	3 (17%)
6	NAG	F	2	6	14,14,15	0.49	0	17,19,21	0.88	0
6	BMA	F	3	6	11,11,12	0.39	0	15,15,17	0.92	1 (6%)
6	BMA	F	4	6	11,11,12	0.32	0	15,15,17	0.67	0
6	BMA	F	5	6	11,11,12	0.40	0	15,15,17	1.62	3 (20%)
5	NAG	G	1	1,5	14,14,15	0.62	0	17,19,21	1.36	1 (5%)
5	NAG	G	2	5	14,14,15	0.57	0	17,19,21	1.37	3 (17%)
5	NAG	H	1	1,5	14,14,15	0.50	0	17,19,21	1.13	2 (11%)
5	NAG	H	2	5	14,14,15	0.53	0	17,19,21	1.22	3 (17%)
5	NAG	I	1	1,5	14,14,15	0.52	0	17,19,21	1.10	1 (5%)
5	NAG	I	2	5	14,14,15	0.73	0	17,19,21	2.23	5 (29%)
5	NAG	J	1	1,5	14,14,15	0.68	0	17,19,21	1.17	2 (11%)
5	NAG	J	2	5	14,14,15	0.49	0	17,19,21	0.74	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	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	1/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	BMA	F	4	6	-	1/2/19/22	0/1/1/1
6	BMA	F	5	6	-	0/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	3/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	5	BMA	C1-O5-C5	4.68	118.53	112.19
5	I	2	NAG	C2-N2-C7	4.62	129.48	122.90
6	F	1	NAG	C1-O5-C5	4.57	118.39	112.19
5	G	1	NAG	C1-O5-C5	4.49	118.27	112.19
5	I	2	NAG	C8-C7-N2	4.09	123.03	116.10
5	I	2	NAG	C4-C3-C2	4.07	116.98	111.02
5	I	2	NAG	C3-C4-C5	3.58	116.62	110.24
5	E	2	NAG	C8-C7-N2	2.87	120.97	116.10
5	E	1	NAG	C4-C3-C2	2.79	115.11	111.02
5	I	2	NAG	O7-C7-C8	-2.76	116.93	122.06
5	J	1	NAG	O5-C5-C4	-2.71	104.23	110.83
5	G	2	NAG	C8-C7-N2	2.60	120.50	116.10
6	F	5	BMA	C3-C4-C5	2.60	114.87	110.24
5	H	2	NAG	C8-C7-N2	2.55	120.42	116.10
6	F	5	BMA	O5-C5-C6	2.44	111.02	107.20
5	E	2	NAG	C2-N2-C7	2.41	126.34	122.90
5	I	1	NAG	C4-C3-C2	2.36	114.48	111.02
5	H	1	NAG	O4-C4-C5	2.23	114.83	109.30
6	F	1	NAG	C8-C7-N2	2.21	119.83	116.10
5	G	2	NAG	C4-C3-C2	2.19	114.23	111.02
5	H	2	NAG	C1-O5-C5	2.19	115.16	112.19
5	G	2	NAG	C3-C4-C5	2.17	114.11	110.24
5	H	2	NAG	C2-N2-C7	2.16	125.98	122.90
5	H	1	NAG	C4-C3-C2	-2.13	107.90	111.02
6	F	3	BMA	C3-C4-C5	2.12	114.02	110.24
6	F	1	NAG	C2-N2-C7	2.03	125.79	122.90
5	J	1	NAG	C3-C4-C5	-2.00	106.67	110.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2

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

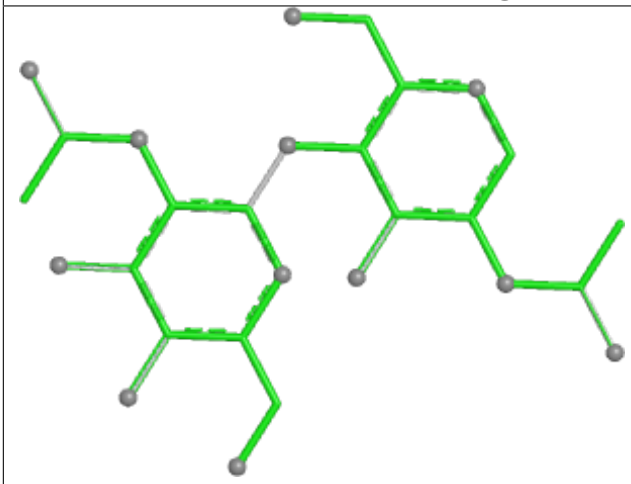
There are no ring outliers.

3 monomers are involved in 3 short contacts:

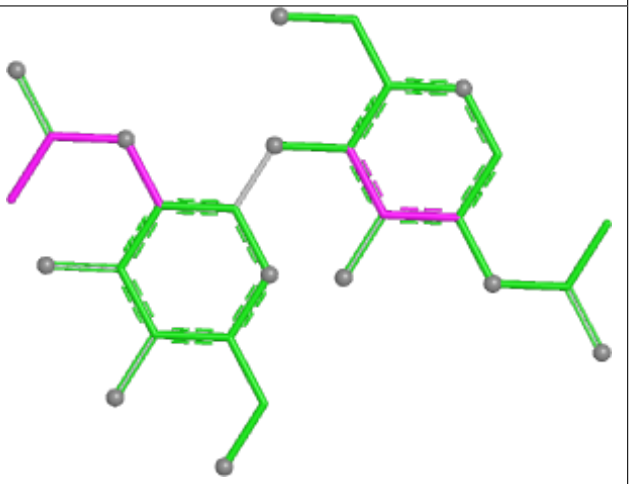
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
5	J	1	NAG	2	0
5	H	1	NAG	1	0

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

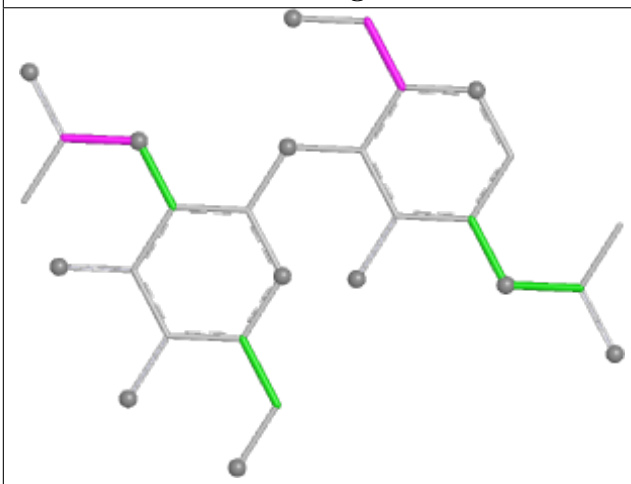
Oligosaccharide Chain E



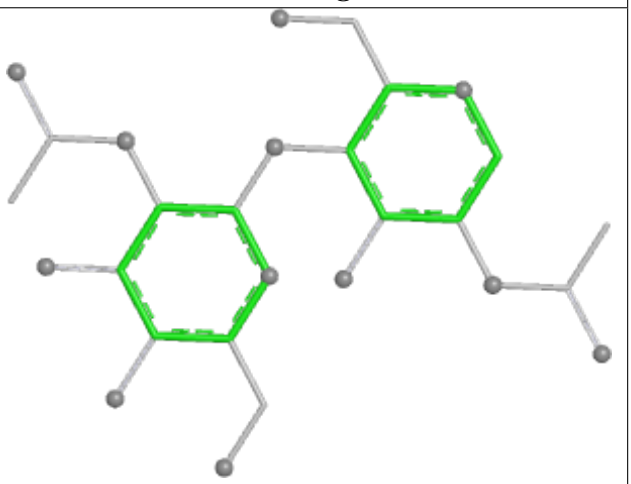
Bond lengths



Bond angles

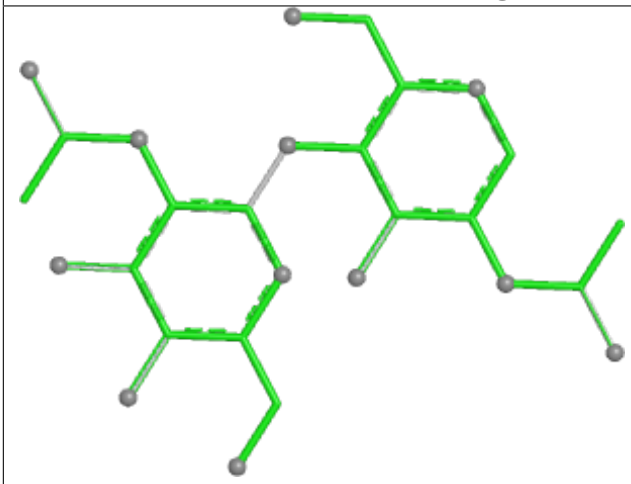


Torsions

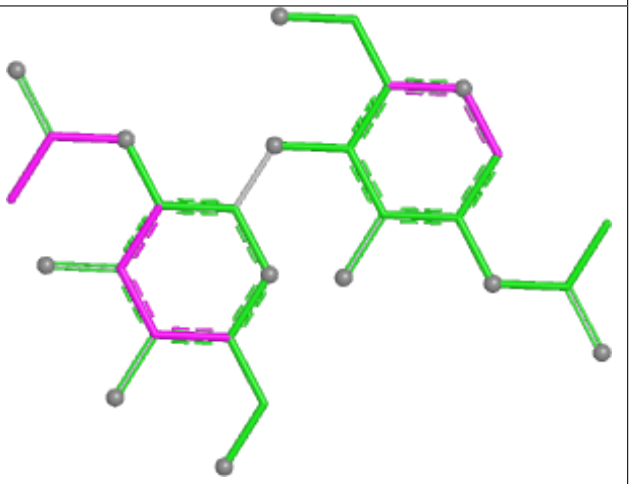


Rings

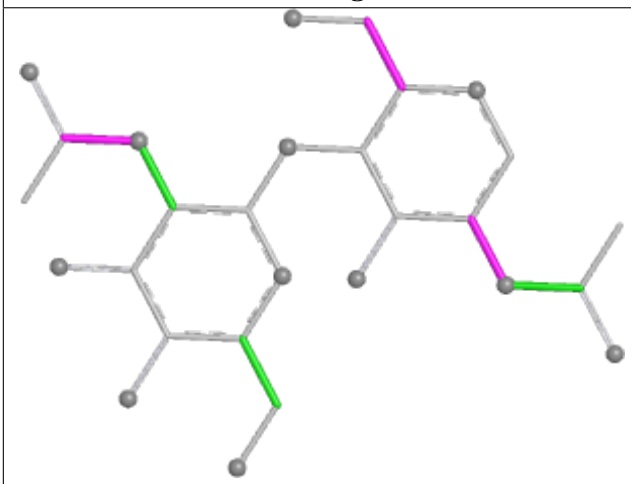
Oligosaccharide Chain G



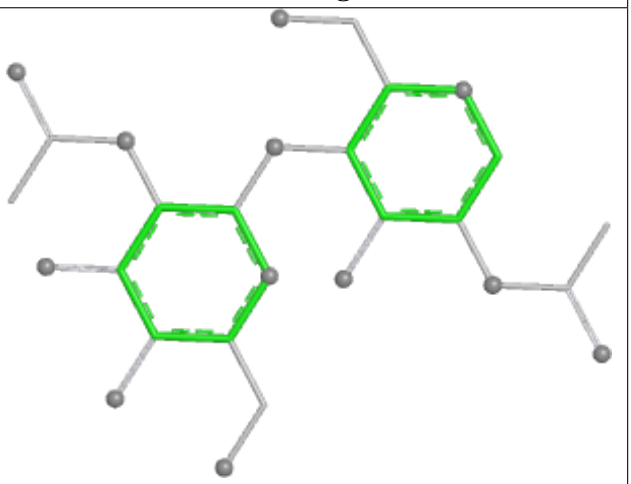
Bond lengths



Bond angles

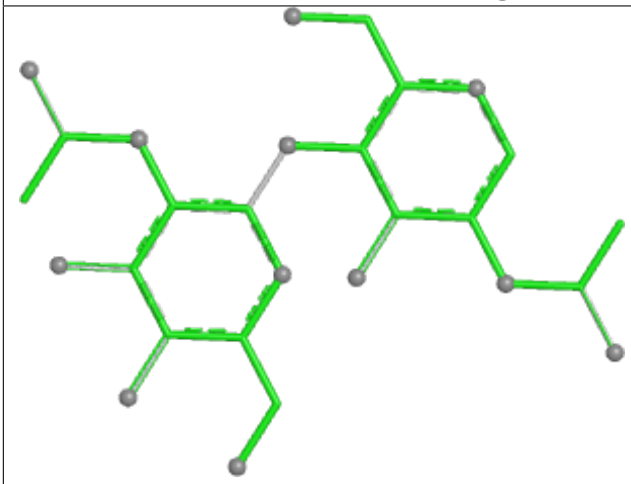


Torsions

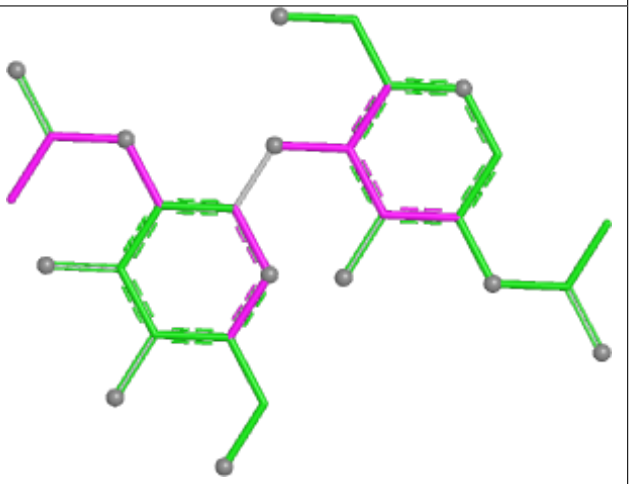


Rings

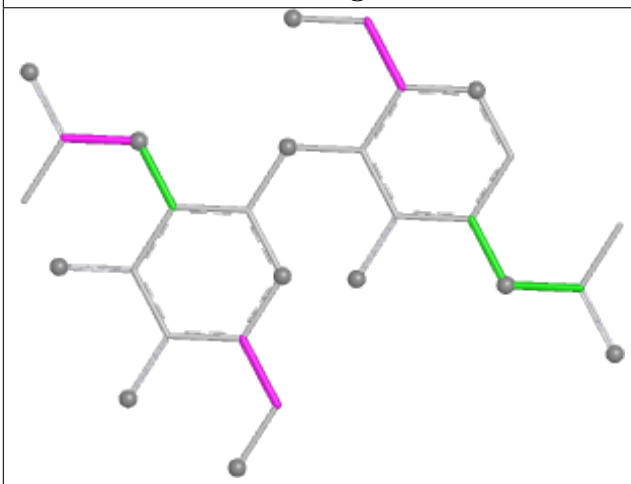
Oligosaccharide Chain H



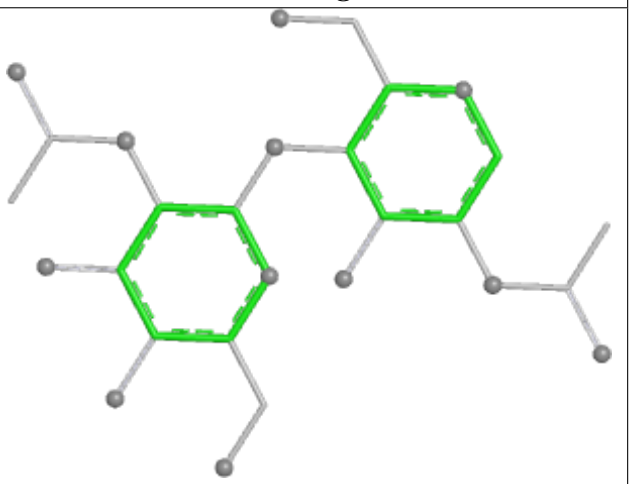
Bond lengths



Bond angles

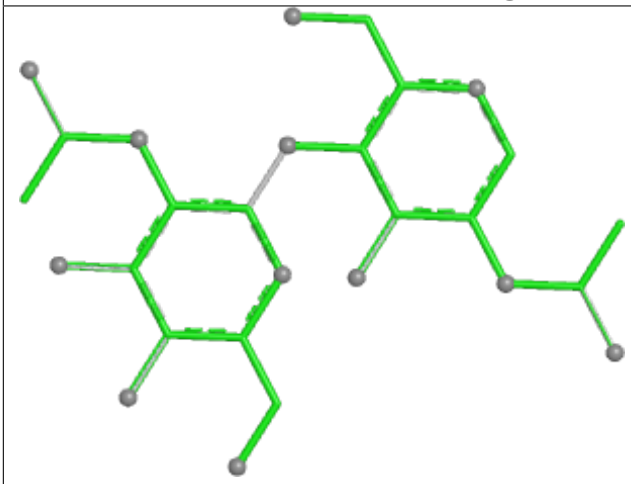


Torsions

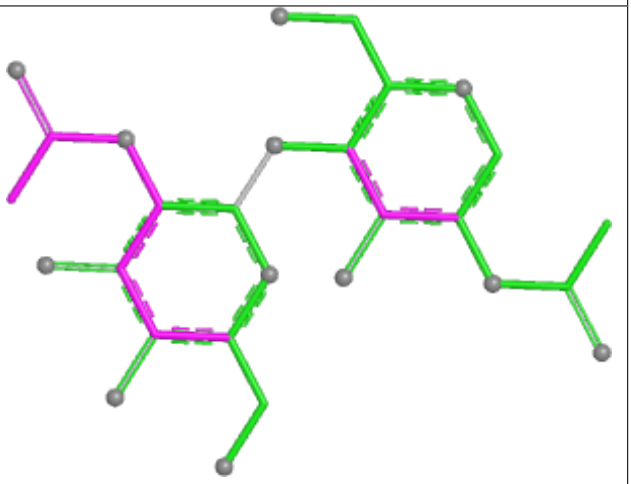


Rings

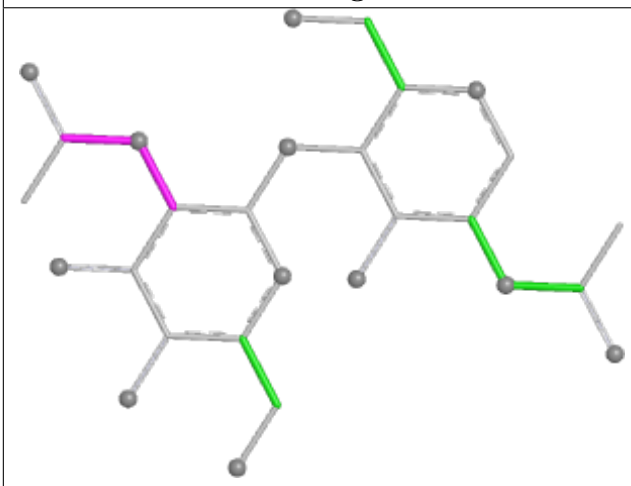
Oligosaccharide Chain I



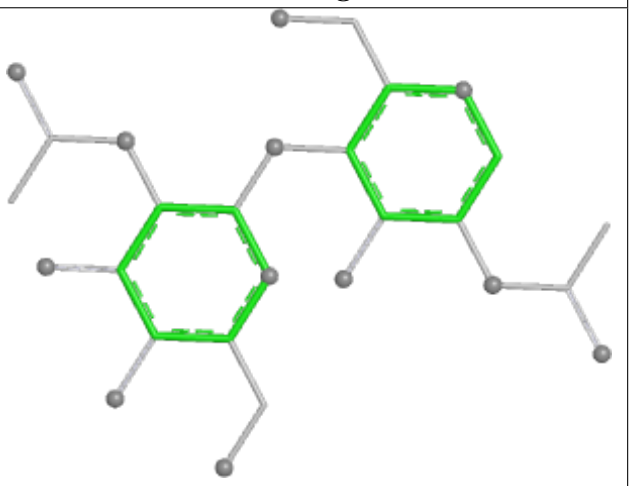
Bond lengths



Bond angles

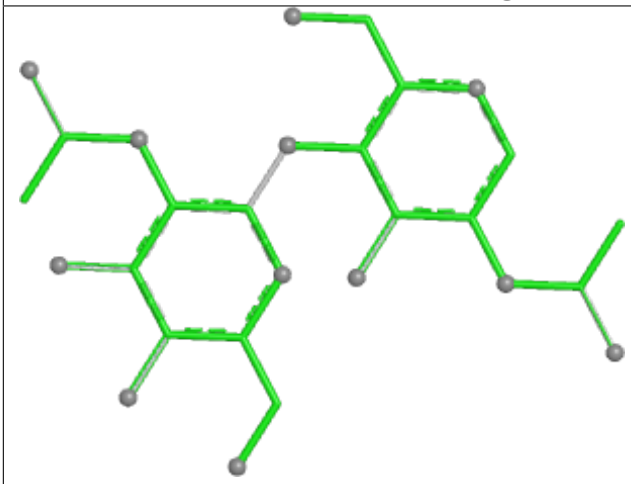


Torsions

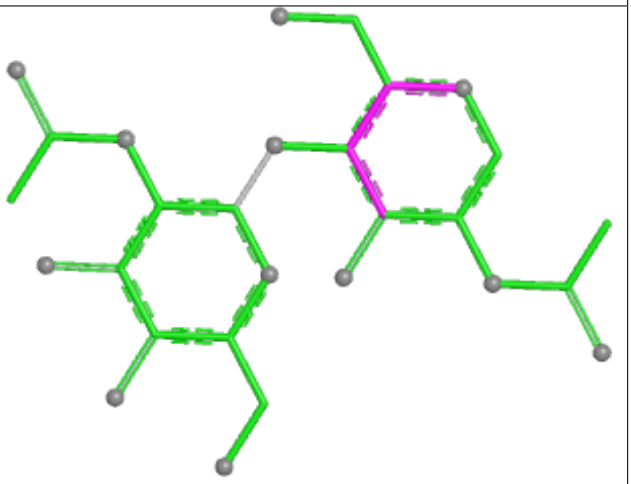


Rings

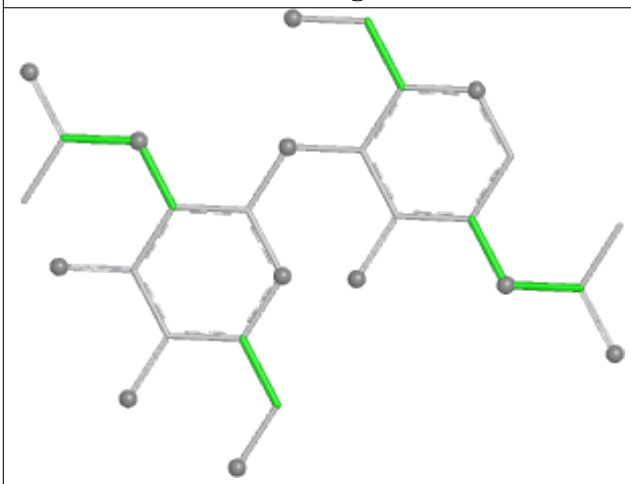
Oligosaccharide Chain J



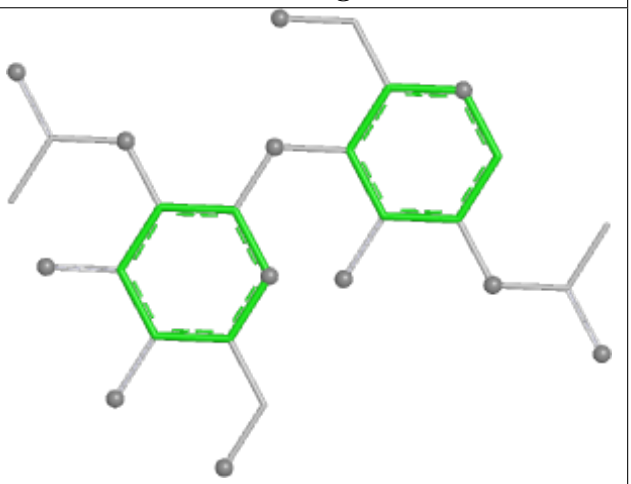
Bond lengths



Bond angles

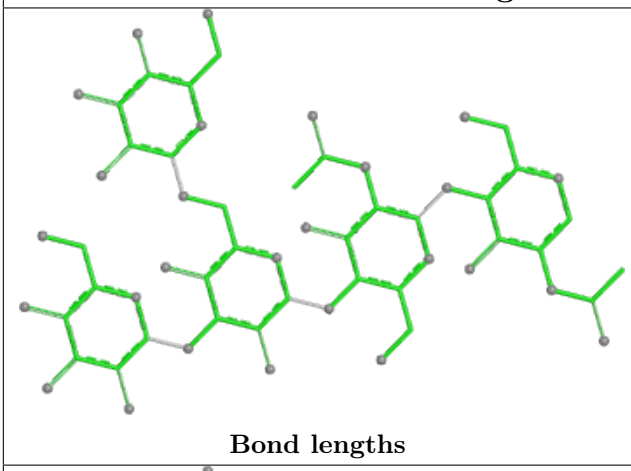


Torsions

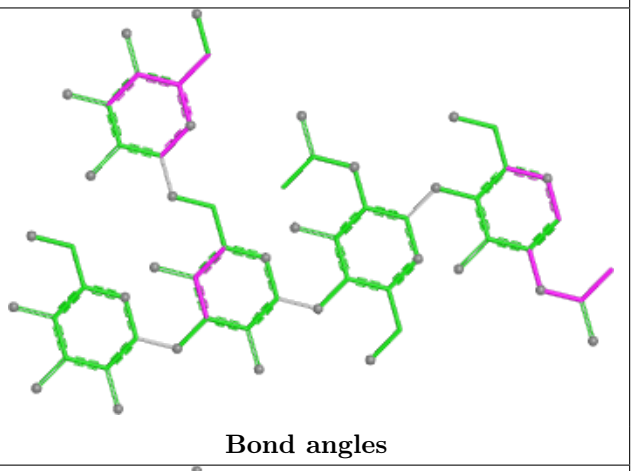


Rings

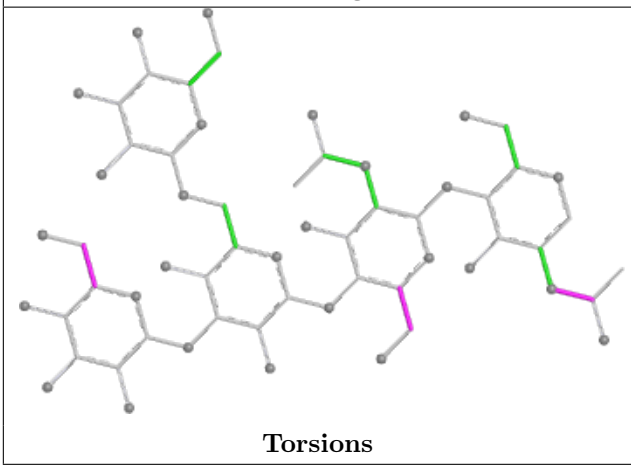
Oligosaccharide Chain F



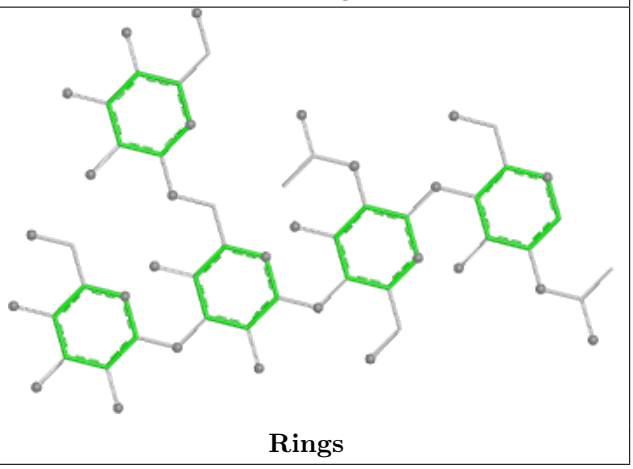
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

7 ligands 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	$\#\|Z\| > 2$
8	PC1	C	1245	-	42,42,53	1.07	2 (4%)	48,50,61	0.97	3 (6%)
7	NAG	A	1715	1	14,14,15	0.48	0	17,19,21	0.88	0
7	NAG	A	1705	1	14,14,15	0.55	0	17,19,21	0.99	1 (5%)
7	NAG	A	1713	1	14,14,15	0.53	0	17,19,21	1.08	1 (5%)
7	NAG	A	1714	1	14,14,15	0.50	0	17,19,21	0.75	0
8	PC1	B	1468	-	42,42,53	1.05	2 (4%)	48,50,61	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	A	1712	1	14,14,15	0.45	0	17,19,21	0.99	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PC1	C	1245	-	-	20/46/46/57	-
7	NAG	A	1715	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1705	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1713	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1714	1	-	0/6/23/26	0/1/1/1
8	PC1	B	1468	-	-	19/46/46/57	-
7	NAG	A	1712	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1245	PC1	O31-C31	4.43	1.46	1.33
8	C	1245	PC1	O21-C21	4.39	1.46	1.34
8	B	1468	PC1	O31-C31	4.33	1.46	1.33
8	B	1468	PC1	O21-C21	4.29	1.46	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1468	PC1	O21-C21-C22	4.07	120.27	111.50
8	C	1245	PC1	O21-C21-C22	3.98	120.08	111.50
7	A	1713	NAG	O5-C1-C2	-2.86	106.78	111.29
7	A	1712	NAG	O5-C1-C2	-2.72	107.00	111.29
8	C	1245	PC1	O31-C31-C32	2.67	120.30	111.91
8	B	1468	PC1	O31-C31-C32	2.54	119.87	111.91
7	A	1705	NAG	O5-C1-C2	-2.24	107.75	111.29
8	C	1245	PC1	O31-C31-O32	-2.08	118.34	123.59

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1245	PC1	C11-O13-P-O11
8	C	1245	PC1	C1-O11-P-O14
8	C	1245	PC1	C1-O11-P-O13
8	C	1245	PC1	O13-C11-C12-N
8	C	1245	PC1	C22-C21-O21-C2
8	B	1468	PC1	O22-C21-O21-C2
8	C	1245	PC1	O22-C21-O21-C2
8	B	1468	PC1	C22-C21-O21-C2
8	B	1468	PC1	C23-C24-C25-C26
8	B	1468	PC1	C27-C28-C29-C2A
8	B	1468	PC1	C34-C35-C36-C37
8	C	1245	PC1	C22-C23-C24-C25
8	C	1245	PC1	C32-C33-C34-C35
8	B	1468	PC1	C36-C37-C38-C39
8	B	1468	PC1	C24-C25-C26-C27
8	C	1245	PC1	C35-C36-C37-C38
8	C	1245	PC1	C32-C31-O31-C3
8	C	1245	PC1	C24-C25-C26-C27
8	C	1245	PC1	O32-C31-O31-C3
8	B	1468	PC1	C21-C22-C23-C24
7	A	1705	NAG	O5-C5-C6-O6
8	B	1468	PC1	C22-C23-C24-C25
8	B	1468	PC1	C31-C32-C33-C34
8	B	1468	PC1	C25-C26-C27-C28
8	B	1468	PC1	C29-C2A-C2B-C2C
8	C	1245	PC1	O11-C1-C2-C3
8	C	1245	PC1	C1-C2-O21-C21
8	B	1468	PC1	O21-C2-C3-O31
8	B	1468	PC1	C2A-C2B-C2C-C2D
8	C	1245	PC1	C2-C1-O11-P
8	C	1245	PC1	C11-O13-P-O14
8	B	1468	PC1	C37-C38-C39-C3A
7	A	1705	NAG	C1-C2-N2-C7
8	B	1468	PC1	C32-C33-C34-C35
8	C	1245	PC1	C26-C27-C28-C29
8	C	1245	PC1	C23-C24-C25-C26
8	B	1468	PC1	O11-C1-C2-O21
7	A	1713	NAG	C4-C5-C6-O6
8	B	1468	PC1	O31-C31-C32-C33
8	C	1245	PC1	C27-C28-C29-C2A
8	C	1245	PC1	C12-C11-O13-P
8	B	1468	PC1	O32-C31-C32-C33

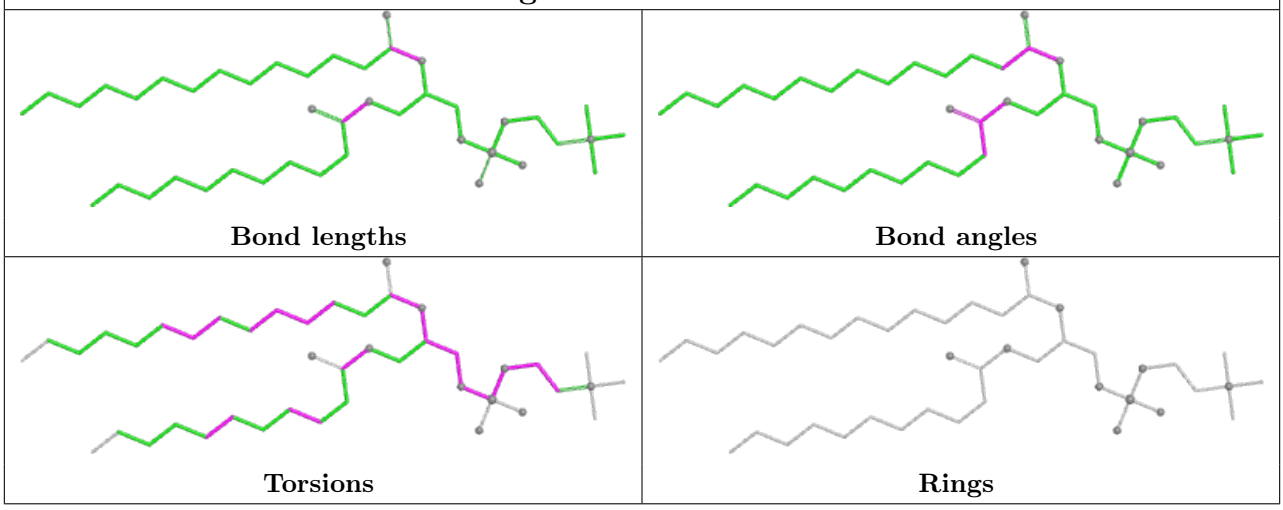
There are no ring outliers.

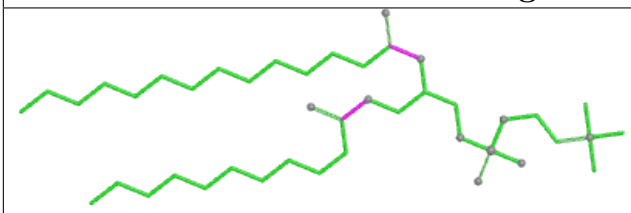
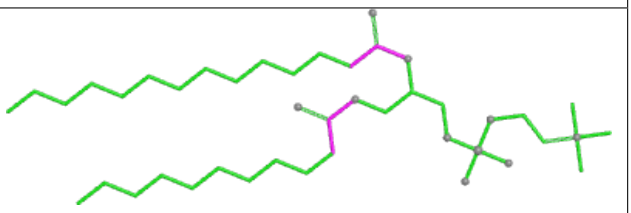
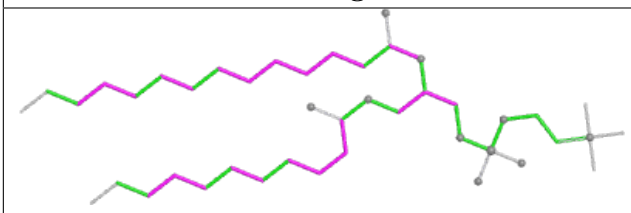
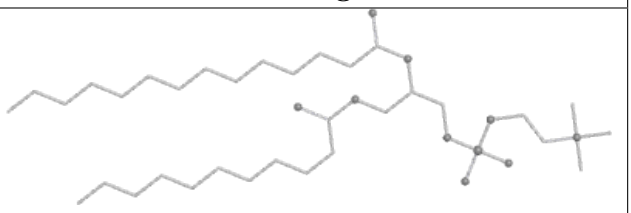
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1245	PC1	1	0
7	A	1705	NAG	2	0
7	A	1714	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PC1 C 1245



Ligand PC1 B 1468	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

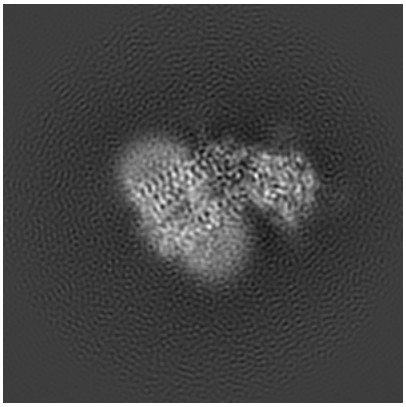
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3061. These allow visual inspection of the internal detail of the map and identification of artifacts.

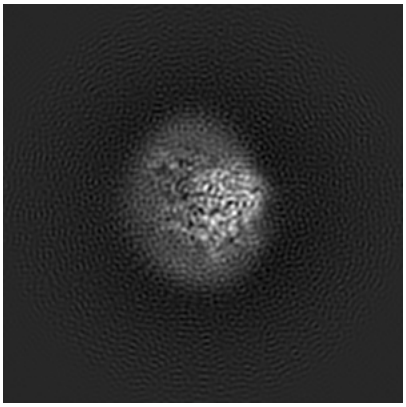
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

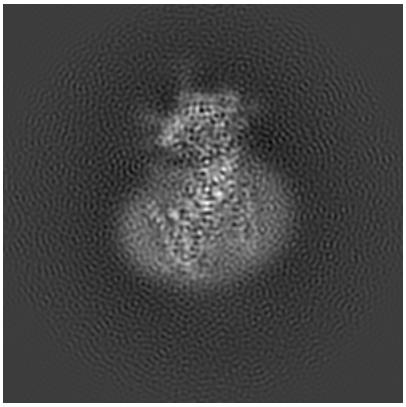
6.1.1 Primary map



X



Y

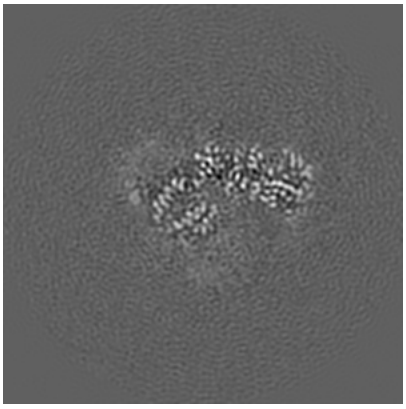


Z

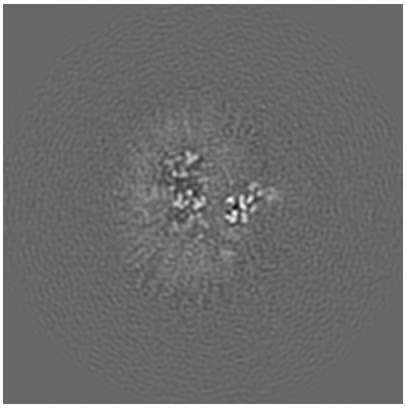
The images above show the map projected in three orthogonal directions.

6.2 Central slices

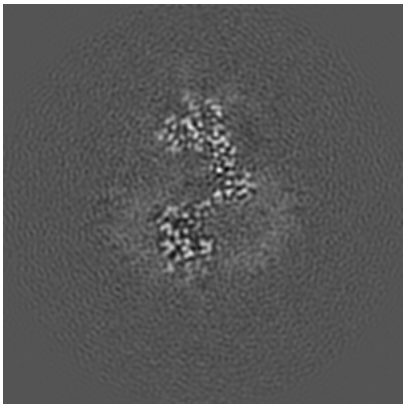
6.2.1 Primary map



X Index: 90



Y Index: 90

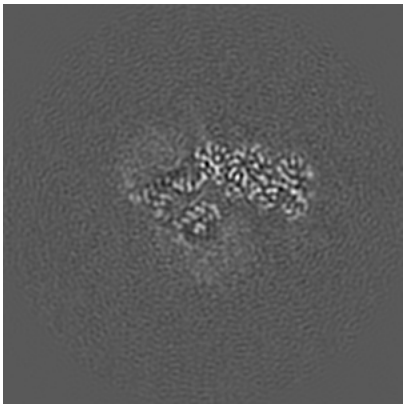


Z Index: 90

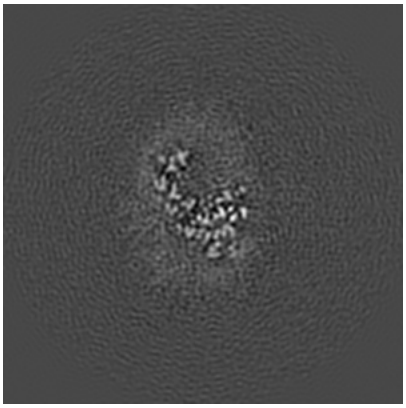
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

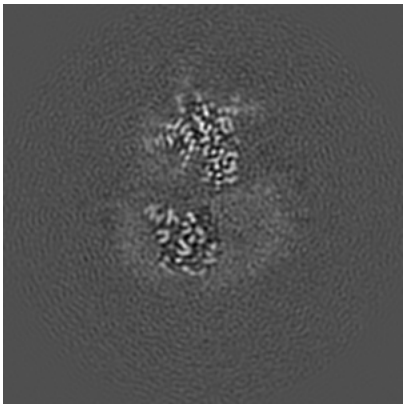
6.3.1 Primary map



X Index: 91



Y Index: 84

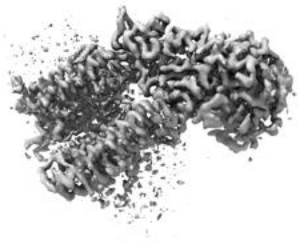


Z Index: 95

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

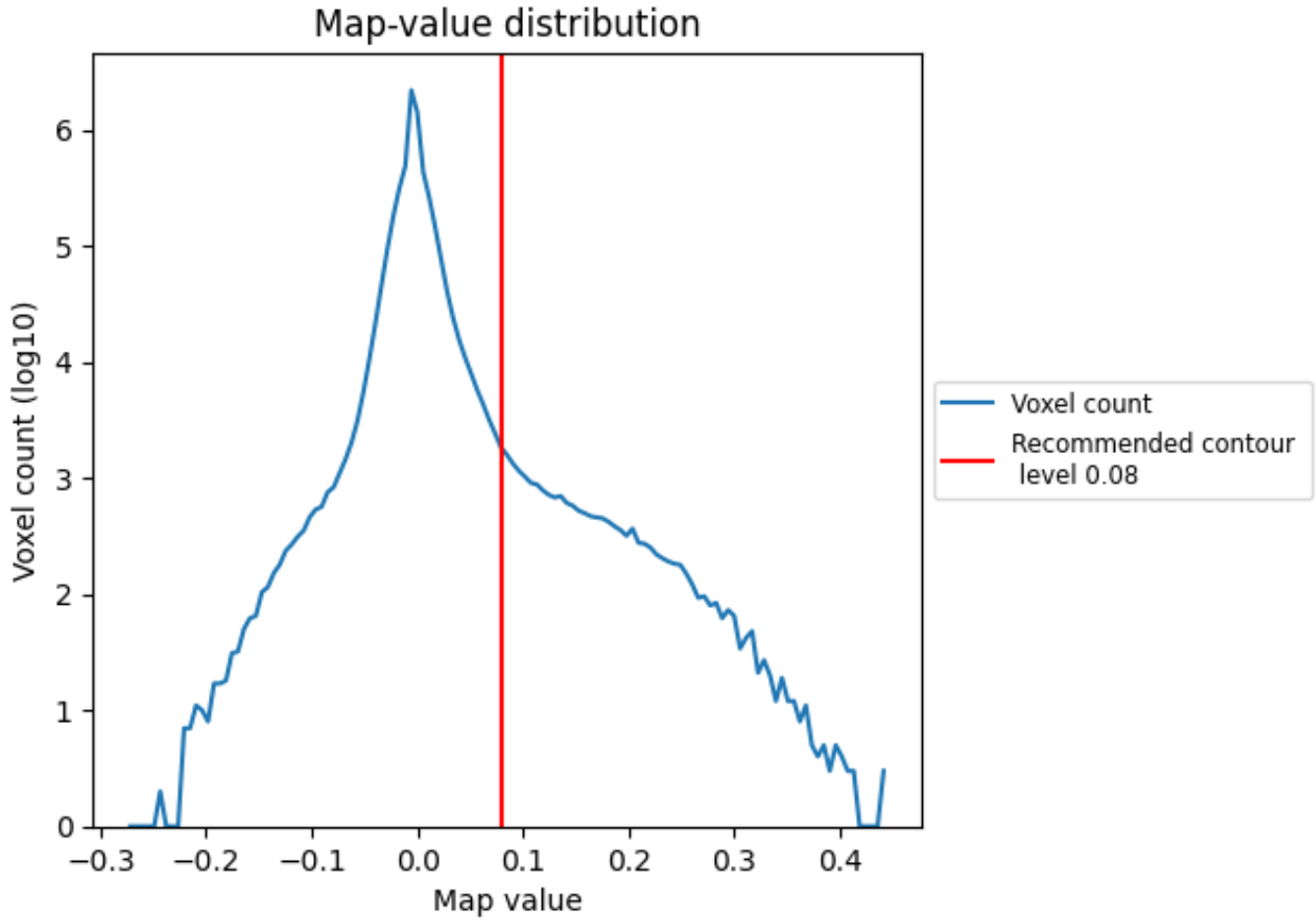
6.5 Mask visualisation (i)

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

7 Map analysis

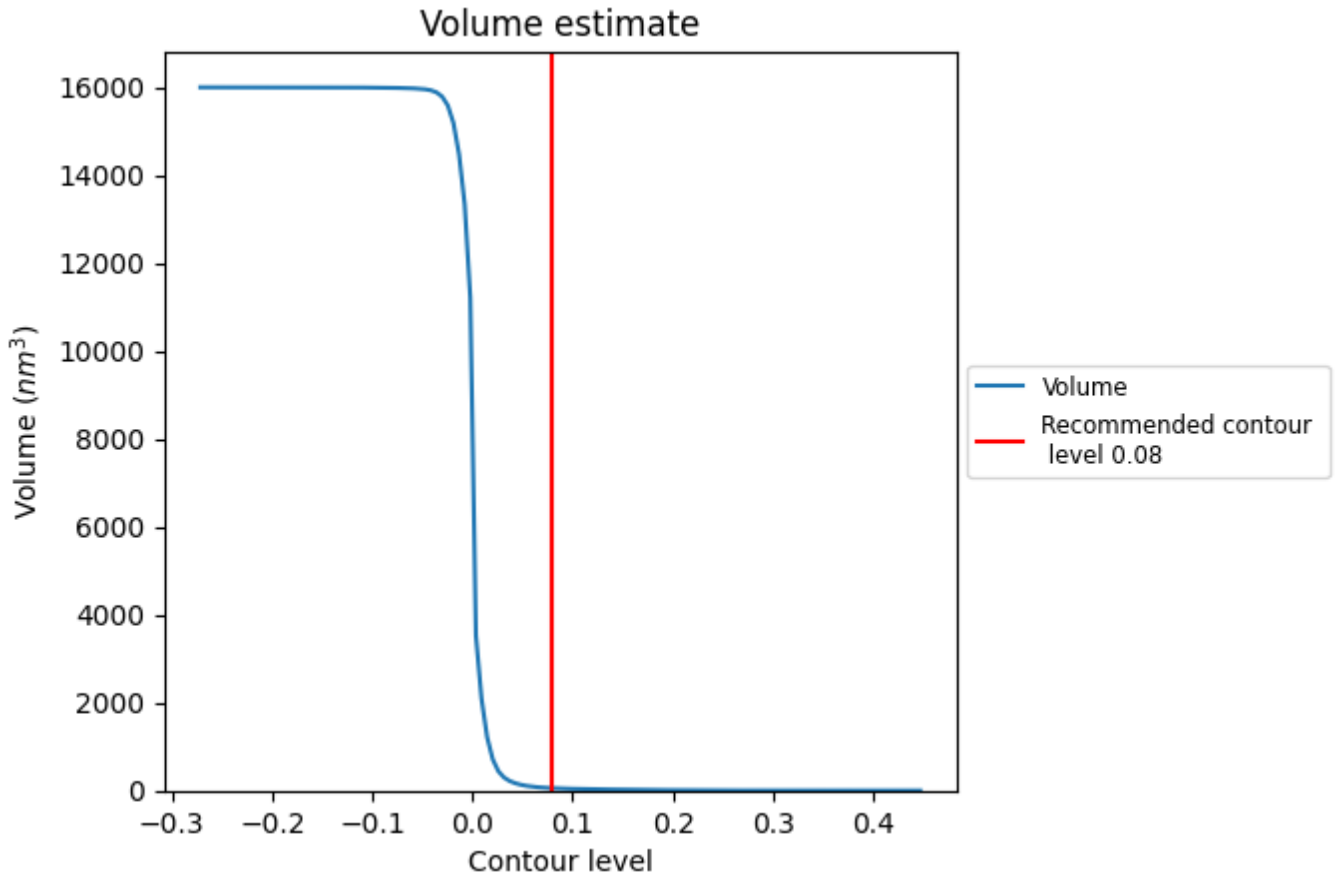
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

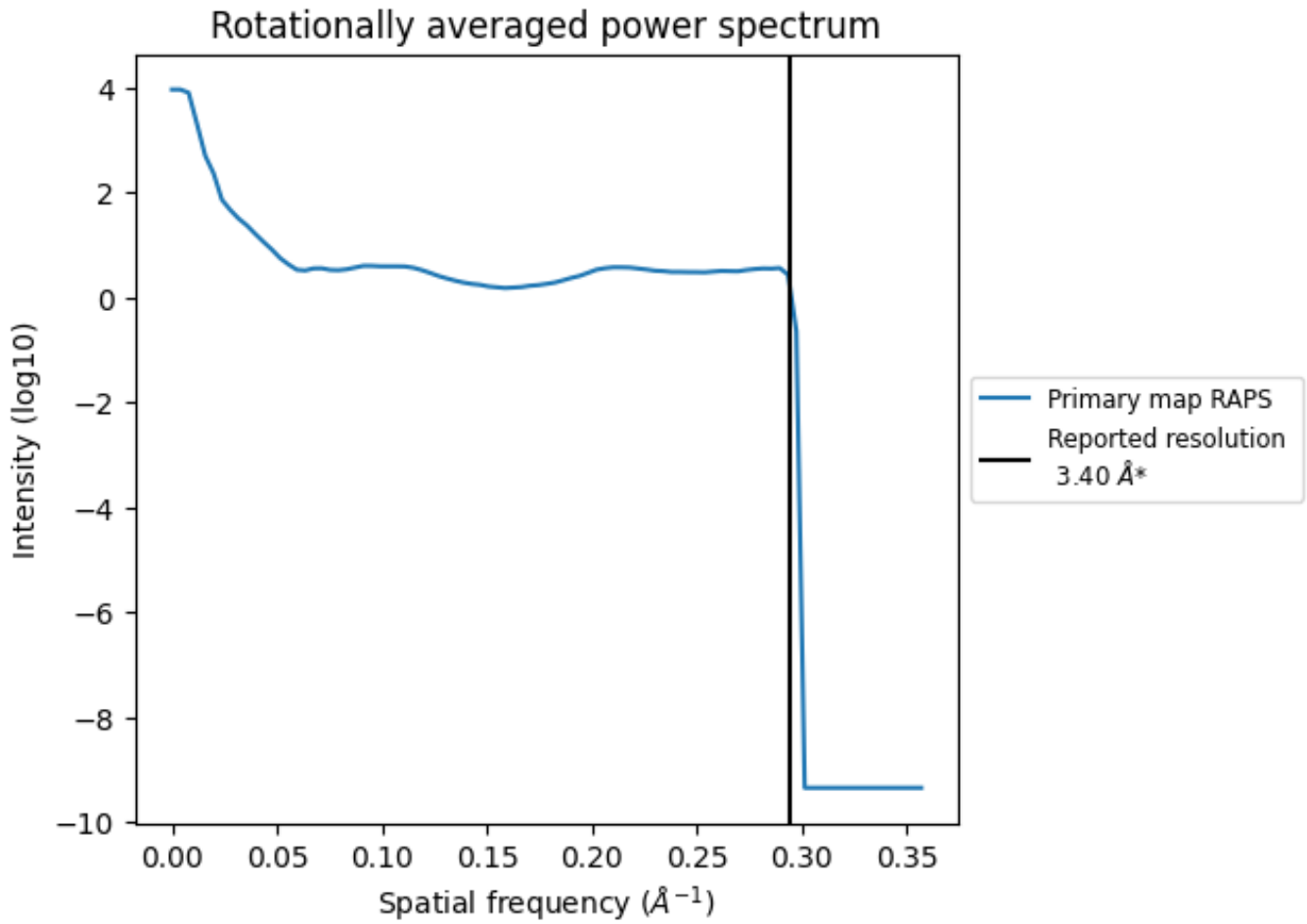
7.2 Volume estimate



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 49 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

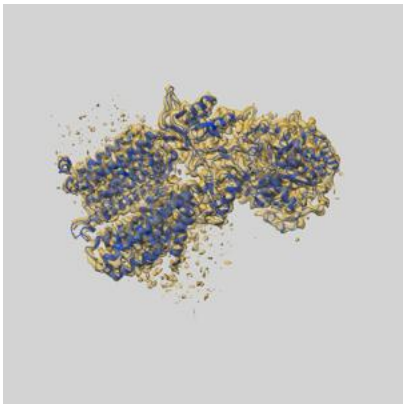
8 Fourier-Shell correlation (i)

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

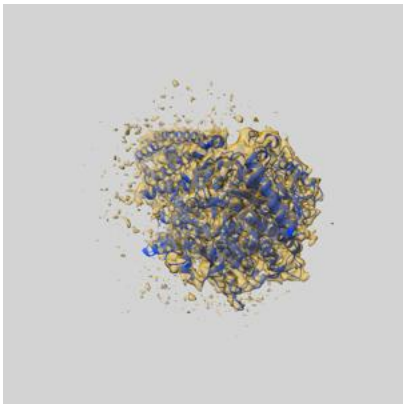
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3061 and PDB model 5A63. Per-residue inclusion information can be found in section 3 on page 7.

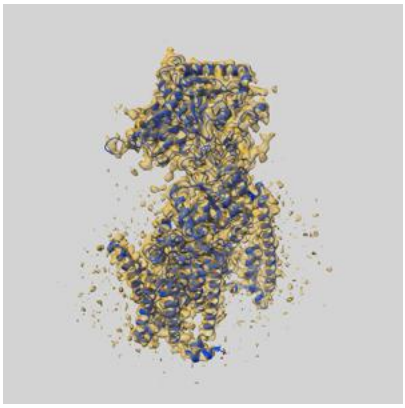
9.1 Map-model overlay



X



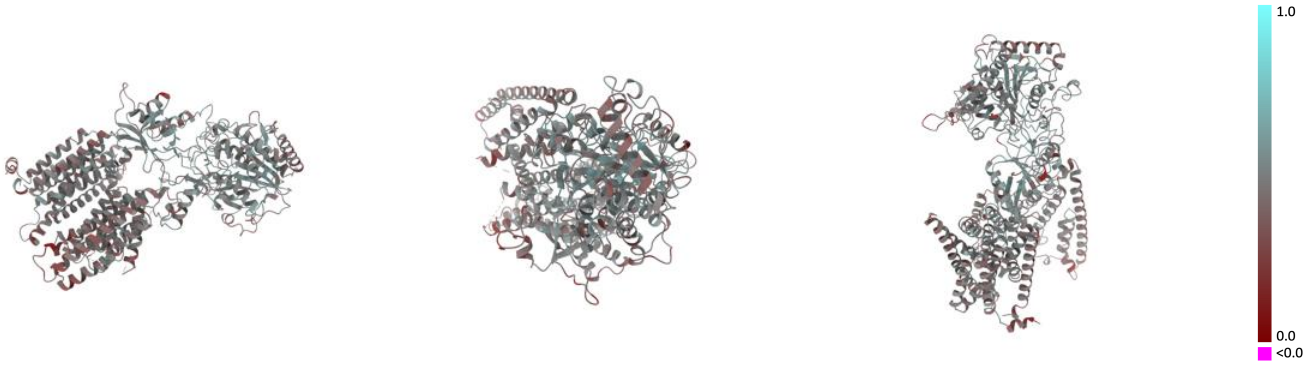
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

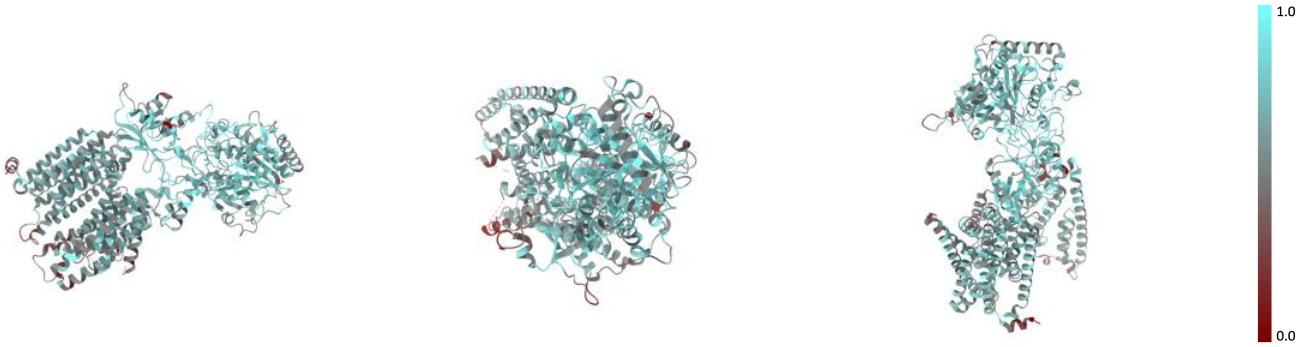
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

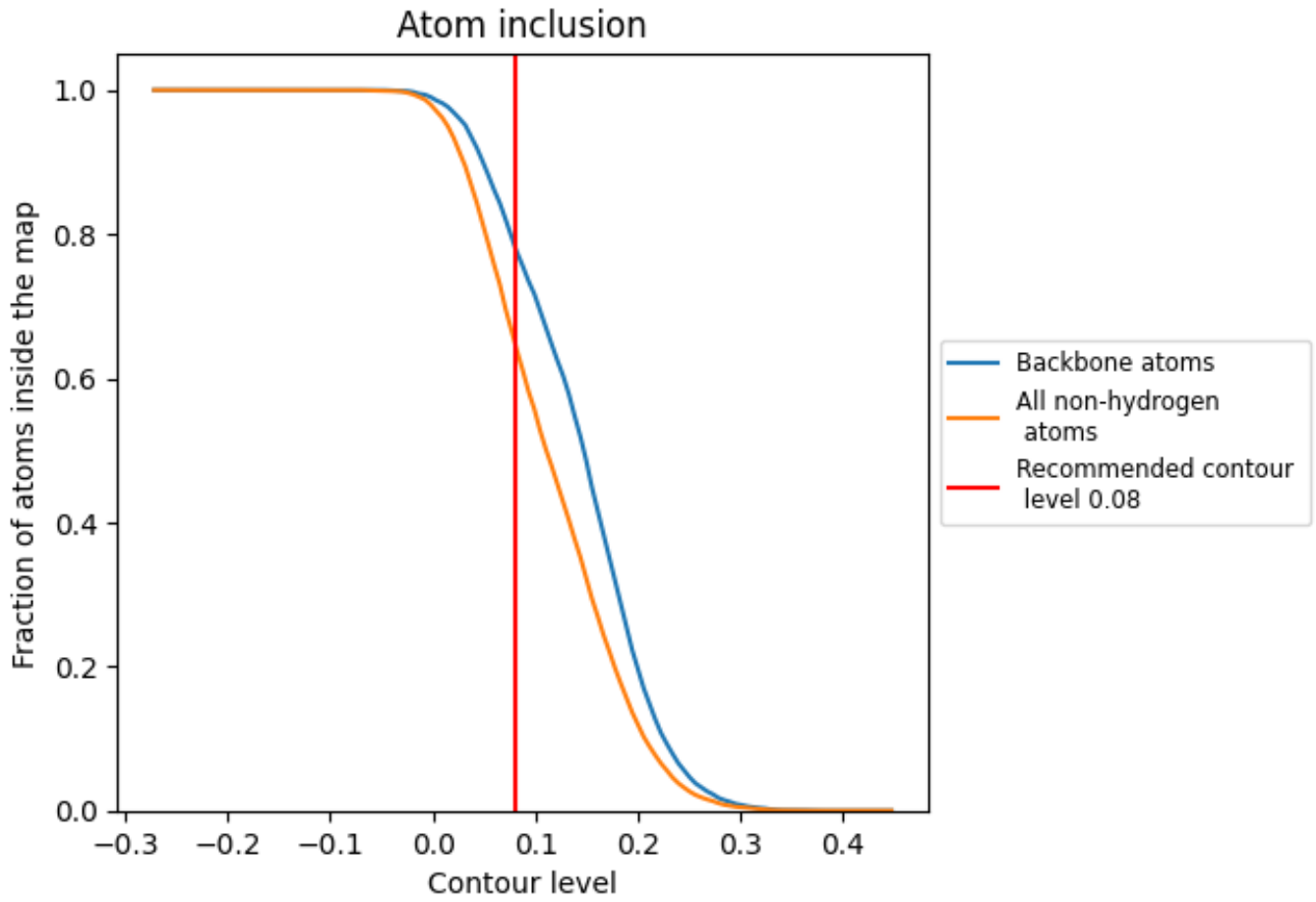
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 65% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6486	0.4570
A	0.6986	0.4780
B	0.5733	0.4410
C	0.6219	0.4480
D	0.5969	0.3980
E	0.5000	0.4230
F	0.5246	0.4320
G	0.6429	0.4040
H	0.5000	0.2720
I	0.2143	0.3160
J	0.3571	0.3160