Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:23 pm GMT

PDB ID	:	9F2J
EMDB ID	:	EMD-50147
Title	:	Cryo-EM structure of SV2B-BoNT/A1 complex
Authors	:	Khanppnavar, B.; Leka, O.; Korkhov, V.; Kammerer, R.
Deposited on	:	2024-04-23
Resolution	:	3.98 Å(reported)
Based on initial models	:	9F2B, 9F1R

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:

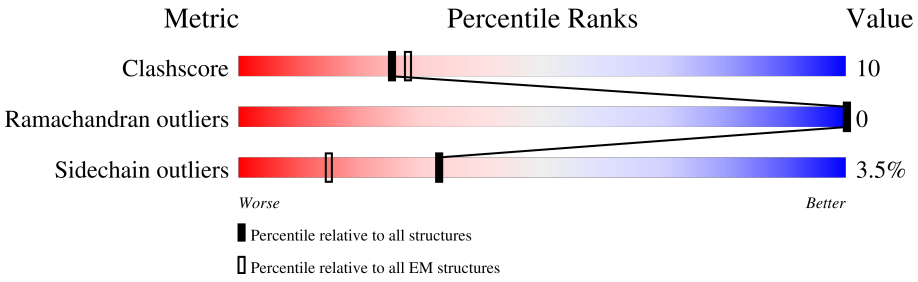
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 3.98 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	1329	74% 19% • 6%
2	A	683	54% 25% • 20%
3	C	2	100%
4	D	6	17% 67% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	C	2	X	-	-	-
4	BMA	D	3	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14646 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1253	10204	6554	1681	1937	32	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P0DPI0
B	-15	ARG	-	expression tag	UNP P0DPI0
B	-14	GLY	-	expression tag	UNP P0DPI0
B	-13	SER	-	expression tag	UNP P0DPI0
B	-12	HIS	-	expression tag	UNP P0DPI0
B	-11	HIS	-	expression tag	UNP P0DPI0
B	-10	HIS	-	expression tag	UNP P0DPI0
B	-9	HIS	-	expression tag	UNP P0DPI0
B	-8	HIS	-	expression tag	UNP P0DPI0
B	-7	HIS	-	expression tag	UNP P0DPI0
B	-6	GLY	-	expression tag	UNP P0DPI0
B	-5	SER	-	expression tag	UNP P0DPI0
B	-4	LEU	-	expression tag	UNP P0DPI0
B	-3	VAL	-	expression tag	UNP P0DPI0
B	-2	PRO	-	expression tag	UNP P0DPI0
B	-1	ARG	-	expression tag	UNP P0DPI0
B	0	GLY	-	expression tag	UNP P0DPI0
B	1	SER	-	expression tag	UNP P0DPI0
B	27	ALA	VAL	variant	UNP P0DPI0
B	224	GLN	GLU	engineered mutation	UNP P0DPI0
B	363	ALA	ARG	engineered mutation	UNP P0DPI0
B	366	PHE	TYR	engineered mutation	UNP P0DPI0
B	1158	ALA	THR	conflict	UNP P0DPI0
B	1297	VAL	-	expression tag	UNP P0DPI0
B	1298	PRO	-	expression tag	UNP P0DPI0
B	1299	PRO	-	expression tag	UNP P0DPI0
B	1300	THR	-	expression tag	UNP P0DPI0
B	1301	PRO	-	expression tag	UNP P0DPI0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1302	GLY	-	expression tag	UNP P0DPI0
B	1303	SER	-	expression tag	UNP P0DPI0
B	1304	ALA	-	expression tag	UNP P0DPI0
B	1305	TRP	-	expression tag	UNP P0DPI0
B	1306	SER	-	expression tag	UNP P0DPI0
B	1307	HIS	-	expression tag	UNP P0DPI0
B	1308	PRO	-	expression tag	UNP P0DPI0
B	1309	GLN	-	expression tag	UNP P0DPI0
B	1310	PHE	-	expression tag	UNP P0DPI0
B	1311	GLU	-	expression tag	UNP P0DPI0
B	1312	LYS	-	expression tag	UNP P0DPI0

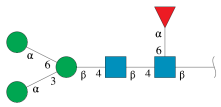
- Molecule 2 is a protein called Synaptic vesicle glycoprotein 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	547	Total	C	N	O	S	0	0
			4333	2844	695	751	43		

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

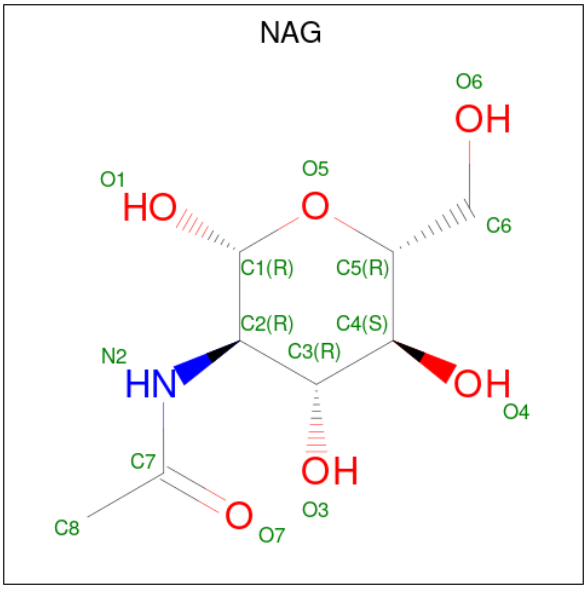
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			24	14	1	9		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



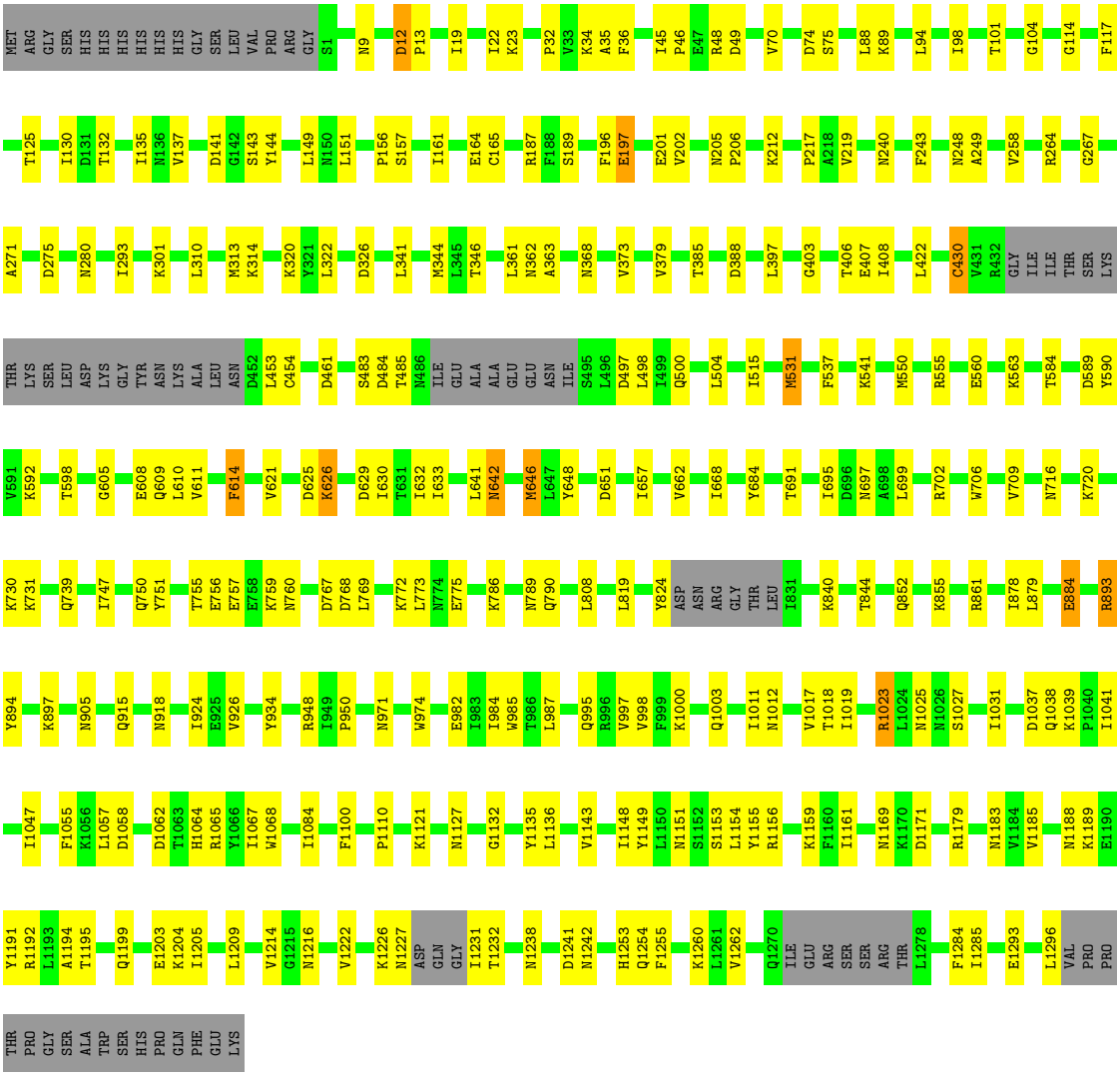
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0

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. 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. 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.

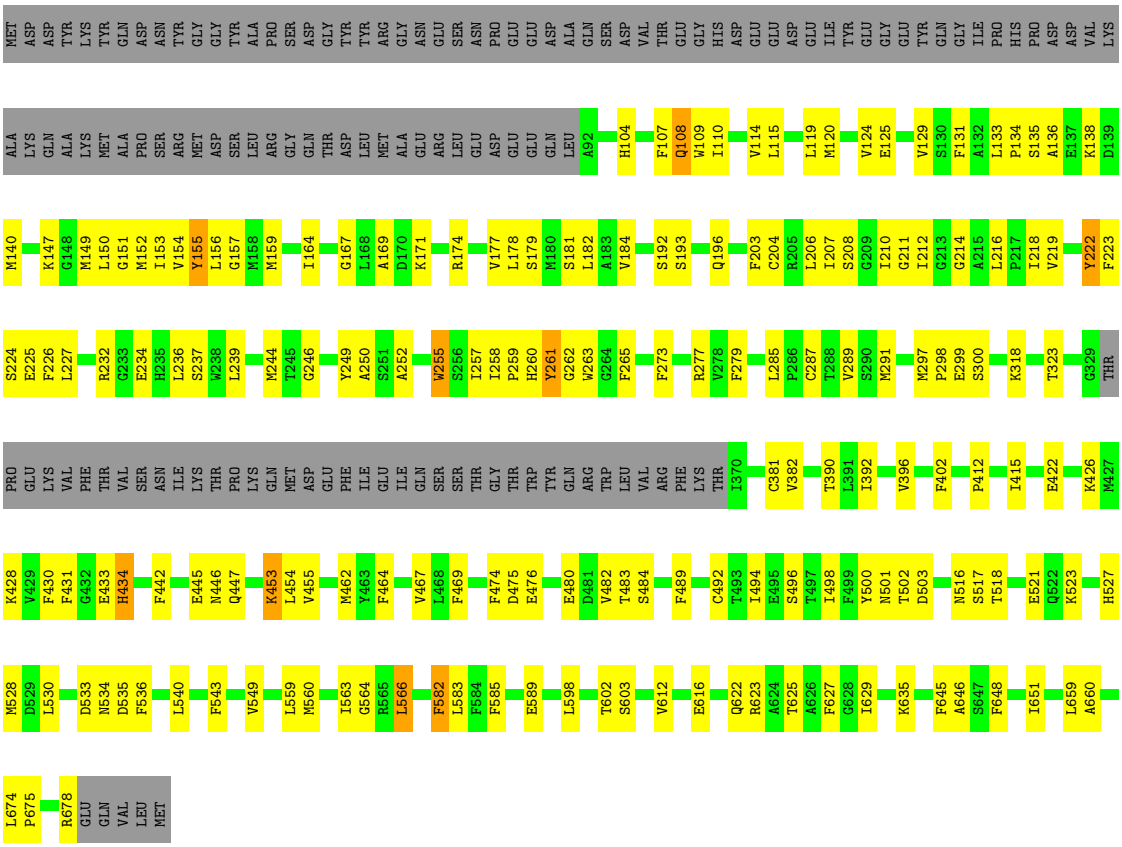
• Molecule 1: Botulinum neurotoxin type A

Chain B:



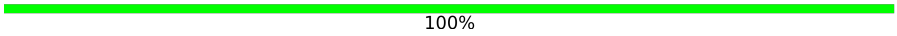
• Molecule 2: Synaptic vesicle glycoprotein 2B

Chain A:



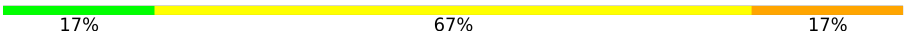
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149718	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, NAG, FUC

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	B	0.29	0/10421	0.49	0/14106
2	A	0.32	0/4451	0.50	1/6014 (0.0%)
All	All	0.30	0/14872	0.49	1/20120 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	583	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1179	ARG	Sidechain

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	B	10204	0	10076	167	0
2	A	4333	0	4279	133	0
3	C	24	0	22	0	0
4	D	71	0	61	10	0
5	A	14	0	13	0	0
All	All	14646	0	14451	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (298) 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)
2:A:516:ASN:HD21	4:D:1:NAG:C1	0.89	1.50
2:A:516:ASN:ND2	4:D:1:NAG:C1	1.74	1.43
1:B:1064:HIS:HB2	4:D:2:NAG:H82	1.50	0.94
1:B:1064:HIS:CB	4:D:2:NAG:H82	1.97	0.93
2:A:434:HIS:HE1	2:A:453:LYS:HE2	1.34	0.91
2:A:516:ASN:HD21	4:D:1:NAG:C2	1.83	0.91
1:B:430:CYS:HB3	1:B:454:CYS:HA	1.57	0.87
2:A:147:LYS:NZ	2:A:646:ALA:HB1	1.91	0.85
1:B:1064:HIS:HB2	4:D:2:NAG:C8	2.06	0.85
2:A:125:GLU:HG3	2:A:212:ILE:HG21	1.58	0.83
2:A:147:LYS:HZ1	2:A:646:ALA:HB1	1.46	0.81
1:B:461:ASP:OD1	1:B:731:LYS:NZ	2.17	0.76
1:B:197:GLU:HG2	1:B:212:LYS:H	1.50	0.76
2:A:222:TYR:OH	2:A:298:PRO:O	2.04	0.75
1:B:1064:HIS:CG	4:D:2:NAG:H82	2.23	0.74
1:B:34:LYS:HG2	1:B:36:PHE:HE1	1.52	0.73
2:A:244:MET:HG3	2:A:549:VAL:HG21	1.72	0.71
2:A:119:LEU:HD12	2:A:239:LEU:HD22	1.71	0.71
2:A:415:ILE:HD11	2:A:589:GLU:HA	1.73	0.71
2:A:434:HIS:CE1	2:A:453:LYS:HE2	2.23	0.70
2:A:147:LYS:HZ1	2:A:646:ALA:CB	2.04	0.70
2:A:516:ASN:ND2	4:D:1:NAG:C2	2.47	0.69
1:B:1159:LYS:HE2	1:B:1185:VAL:HG21	1.74	0.69
1:B:135:ILE:HD13	1:B:149:LEU:HD13	1.74	0.69
2:A:560:MET:HE1	2:A:612:VAL:HG21	1.75	0.68
2:A:516:ASN:CG	4:D:1:NAG:C1	2.62	0.68
1:B:1003:GLN:O	1:B:1151:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:232:ARG:HH11	2:A:616:GLU:HG2	1.59	0.67
1:B:201:GLU:OE1	1:B:205:ASN:ND2	2.28	0.67
2:A:120:MET:HG3	2:A:246:GLY:HA2	1.77	0.67
2:A:428:LYS:HB3	2:A:447:GLN:HE21	1.59	0.67
1:B:610:LEU:HD12	1:B:747:ILE:HD11	1.77	0.66
2:A:151:GLY:O	2:A:154:VAL:HG12	1.98	0.64
1:B:22:ILE:HG22	1:B:137:VAL:HG12	1.79	0.63
1:B:1161:ILE:HG12	1:B:1183:ASN:HB2	1.80	0.63
1:B:756:GLU:OE2	1:B:759:LYS:NZ	2.30	0.62
2:A:462:MET:HG2	2:A:482:VAL:HG23	1.81	0.62
1:B:1023:ARG:HH21	1:B:1047:ILE:HG12	1.65	0.62
2:A:257:ILE:HG22	2:A:258:ILE:HG23	1.82	0.61
1:B:982:GLU:OE2	1:B:1000:LYS:NZ	2.32	0.61
1:B:1121:LYS:HD3	1:B:1136:LEU:HB3	1.82	0.61
1:B:614:PHE:HD2	1:B:773:LEU:HD22	1.64	0.61
2:A:426:LYS:O	2:A:446:ASN:ND2	2.33	0.61
2:A:138:LYS:HB3	2:A:261:TYR:HD2	1.64	0.60
1:B:1296:LEU:HD22	2:A:498:ILE:HG21	1.83	0.60
1:B:756:GLU:O	1:B:760:ASN:ND2	2.34	0.60
2:A:149:MET:HB3	2:A:152:MET:HG3	1.85	0.59
2:A:181:SER:OG	2:A:211:GLY:O	2.18	0.59
1:B:310:LEU:HD21	1:B:314:LYS:HE3	1.85	0.59
2:A:489:PHE:HB3	2:A:492:CYS:SG	2.42	0.59
1:B:156:PRO:HD3	1:B:189:SER:HB2	1.85	0.58
1:B:1227:ASN:HB2	1:B:1231:ILE:HG23	1.85	0.58
1:B:584:THR:OG1	1:B:739:GLN:NE2	2.36	0.58
2:A:131:PHE:HE2	2:A:412:PRO:HG2	1.69	0.58
1:B:48:ARG:NH2	1:B:157:SER:O	2.37	0.58
1:B:657:ILE:HG21	1:B:884:GLU:HG2	1.86	0.58
1:B:313:MET:HE1	1:B:515:ILE:HD12	1.85	0.57
1:B:1194:ALA:HB3	1:B:1209:LEU:HD12	1.88	0.56
1:B:1296:LEU:HD22	2:A:498:ILE:HD13	1.88	0.56
1:B:589:ASP:OD1	1:B:590:TYR:N	2.39	0.56
2:A:674:LEU:HD12	2:A:675:PRO:HD2	1.88	0.56
1:B:1222:VAL:HG13	1:B:1238:ASN:HB3	1.87	0.55
2:A:433:GLU:N	2:A:433:GLU:OE2	2.40	0.55
1:B:46:PRO:HG3	1:B:88:LEU:HD13	1.88	0.55
2:A:147:LYS:NZ	2:A:646:ALA:CB	2.66	0.55
2:A:152:MET:O	2:A:155:TYR:HB2	2.07	0.55
2:A:225:GLU:OE1	2:A:623:ARG:NH1	2.40	0.55
1:B:699:LEU:HD13	1:B:844:THR:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:THR:HG23	1:B:388:ASP:H	1.72	0.55
1:B:1003:GLN:HA	1:B:1011:ILE:HD11	1.87	0.55
1:B:1214:VAL:HG12	1:B:1216:ASN:H	1.71	0.55
2:A:517:SER:OG	2:A:518:THR:N	2.37	0.55
1:B:974:TRP:HB3	1:B:987:LEU:HD12	1.89	0.55
1:B:101:THR:HG22	1:B:104:GLY:H	1.72	0.55
1:B:598:THR:O	1:B:750:GLN:NE2	2.39	0.55
2:A:422:GLU:O	2:A:426:LYS:NZ	2.40	0.54
1:B:49:ASP:OD2	1:B:187:ARG:NE	2.28	0.54
1:B:407:GLU:HG3	1:B:408:ILE:HD12	1.89	0.54
1:B:422:LEU:HD23	1:B:422:LEU:H	1.71	0.54
2:A:563:ILE:HD12	2:A:563:ILE:H	1.72	0.54
1:B:161:ILE:HG12	1:B:161:ILE:O	2.07	0.54
1:B:74:ASP:OD1	1:B:75:SER:N	2.41	0.54
1:B:89:LYS:HB2	1:B:379:VAL:HG22	1.89	0.53
1:B:1064:HIS:HB2	4:D:2:NAG:H81	1.89	0.53
2:A:136:ALA:HB2	2:A:263:TRP:CZ2	2.43	0.53
2:A:476:GLU:HG3	2:A:476:GLU:O	2.08	0.53
2:A:603:SER:O	2:A:603:SER:OG	2.21	0.53
2:A:167:GLY:HA2	2:A:625:THR:HA	1.91	0.53
2:A:402:PHE:CZ	2:A:659:LEU:HD21	2.44	0.53
1:B:23:LYS:HD3	1:B:32:PRO:HG3	1.90	0.52
2:A:454:LEU:HD22	2:A:474:PHE:HE1	1.75	0.52
2:A:120:MET:HG3	2:A:246:GLY:CA	2.40	0.52
1:B:948:ARG:HB3	1:B:1068:TRP:HB2	1.91	0.52
1:B:12:ASP:HB2	1:B:19:ILE:HD12	1.91	0.51
1:B:1255:PHE:HB3	1:B:1260:LYS:HD2	1.92	0.51
2:A:259:PRO:O	2:A:260:HIS:ND1	2.43	0.51
2:A:120:MET:O	2:A:124:VAL:HG13	2.10	0.51
1:B:995:GLN:NE2	1:B:1039:LYS:HB3	2.25	0.51
2:A:115:LEU:HD22	2:A:219:VAL:HG23	1.93	0.51
1:B:1199:GLN:HE21	1:B:1204:LYS:HA	1.76	0.51
1:B:19:ILE:HG23	1:B:36:PHE:CD1	2.46	0.51
2:A:412:PRO:O	2:A:415:ILE:HG22	2.11	0.50
1:B:164:GLU:OE2	1:B:187:ARG:NH1	2.44	0.50
1:B:212:LYS:O	1:B:406:THR:HG22	2.11	0.50
1:B:362:ASN:OD1	1:B:363:ALA:N	2.43	0.50
1:B:878:ILE:HG13	1:B:894:TYR:CD2	2.46	0.50
1:B:1183:ASN:OD1	1:B:1192:ARG:NH1	2.45	0.50
2:A:299:GLU:OE1	2:A:300:SER:N	2.30	0.50
2:A:625:THR:O	2:A:629:ILE:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:HG11	1:B:362:ASN:HD22	1.77	0.50
1:B:70:VAL:HG22	1:B:373:VAL:HG23	1.94	0.50
2:A:174:ARG:HG2	2:A:174:ARG:HH11	1.75	0.50
2:A:483:THR:HG23	2:A:527:HIS:HB2	1.94	0.50
1:B:789:ASN:HD21	1:B:861:ARG:HD2	1.76	0.49
2:A:107:PHE:HB2	2:A:323:THR:HG21	1.94	0.49
2:A:464:PHE:HE2	2:A:469:PHE:HE2	1.60	0.49
2:A:138:LYS:O	2:A:262:GLY:HA2	2.11	0.49
2:A:415:ILE:HD11	2:A:589:GLU:HG2	1.93	0.49
1:B:550:MET:HB2	1:B:641:LEU:HB3	1.94	0.49
2:A:483:THR:CG2	2:A:527:HIS:HB2	2.42	0.49
2:A:125:GLU:HG2	2:A:212:ILE:HD13	1.95	0.49
1:B:267:GLY:HA2	1:B:271:ALA:HB2	1.95	0.48
1:B:94:LEU:HD11	1:B:217:PRO:HB2	1.96	0.48
1:B:397:LEU:HD23	1:B:403:GLY:HA2	1.95	0.48
1:B:924:ILE:HB	1:B:1055:PHE:HB2	1.94	0.48
1:B:1203:GLU:OE1	1:B:1203:GLU:HA	2.13	0.48
2:A:261:TYR:HD1	2:A:261:TYR:H	1.62	0.48
2:A:114:VAL:HG21	2:A:297:MET:HG3	1.95	0.48
1:B:19:ILE:HG23	1:B:36:PHE:CE1	2.49	0.48
2:A:203:PHE:O	2:A:207:ILE:HG22	2.13	0.47
2:A:442:PHE:O	2:A:462:MET:HB2	2.14	0.47
2:A:169:ALA:HB2	2:A:177:VAL:HG11	1.95	0.47
2:A:179:SER:HA	2:A:291:MET:HE1	1.97	0.47
1:B:483:SER:N	1:B:684:TYR:OH	2.47	0.47
1:B:702:ARG:HH21	1:B:844:THR:HG22	1.78	0.47
2:A:110:ILE:O	2:A:114:VAL:HG13	2.13	0.47
1:B:485:THR:H	1:B:697:ASN:ND2	2.12	0.47
1:B:1189:LYS:NZ	1:B:1191:TYR:OH	2.47	0.47
2:A:382:VAL:HA	2:A:390:THR:HG21	1.96	0.47
1:B:751:TYR:CE1	1:B:759:LYS:HG2	2.49	0.47
2:A:171:LYS:HA	2:A:171:LYS:HD3	1.70	0.47
2:A:453:LYS:HB3	2:A:453:LYS:HE3	1.45	0.47
2:A:536:PHE:CE2	2:A:540:LEU:HD12	2.50	0.47
1:B:1195:THR:OG1	1:B:1205:ILE:O	2.28	0.47
2:A:318:LYS:HE2	2:A:318:LYS:HB3	1.63	0.47
1:B:948:ARG:NH1	1:B:1012:ASN:OD1	2.48	0.47
1:B:629:ASP:OD1	1:B:790:GLN:NE2	2.48	0.46
1:B:852:GLN:HG3	1:B:855:LYS:HD3	1.97	0.46
1:B:555:ARG:O	1:B:555:ARG:NH1	2.49	0.46
1:B:662:VAL:HG13	1:B:668:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:LEU:HD23	1:B:819:LEU:HA	1.77	0.46
2:A:428:LYS:HB2	2:A:447:GLN:HG2	1.98	0.46
2:A:431:PHE:N	2:A:433:GLU:OE1	2.49	0.46
1:B:243:PHE:HB3	1:B:258:VAL:HG13	1.98	0.46
1:B:840:LYS:O	1:B:844:THR:OG1	2.21	0.46
2:A:502:THR:O	2:A:523:LYS:N	2.49	0.46
2:A:564:GLY:HA2	2:A:678:ARG:HD2	1.96	0.46
1:B:950:PRO:HG2	1:B:1065:ARG:HH11	1.80	0.46
1:B:1017:VAL:HG22	1:B:1031:ILE:HD12	1.98	0.46
1:B:531:MET:SD	1:B:531:MET:N	2.88	0.46
1:B:1110:PRO:HB2	1:B:1159:LYS:HE3	1.98	0.46
2:A:124:VAL:HG12	2:A:250:ALA:HB2	1.98	0.46
1:B:560:GLU:OE1	1:B:560:GLU:N	2.42	0.46
1:B:879:LEU:HD21	1:B:926:VAL:HG11	1.98	0.46
2:A:234:GLU:O	2:A:237:SER:OG	2.26	0.46
2:A:483:THR:HA	2:A:503:ASP:OD2	2.15	0.46
1:B:114:GLY:HA2	1:B:320:LYS:HG3	1.97	0.46
1:B:125:THR:O	1:B:125:THR:OG1	2.30	0.46
1:B:196:PHE:HZ	1:B:361:LEU:HB3	1.80	0.46
2:A:147:LYS:HZ3	2:A:646:ALA:HB1	1.78	0.46
2:A:138:LYS:HB2	2:A:261:TYR:HB2	1.99	0.45
2:A:476:GLU:OE1	2:A:496:SER:O	2.34	0.45
2:A:645:PHE:HZ	2:A:660:ALA:HB2	1.81	0.45
1:B:36:PHE:HD2	1:B:88:LEU:HD21	1.81	0.45
2:A:115:LEU:HB3	2:A:219:VAL:HG23	1.97	0.45
2:A:530:LEU:HA	2:A:533:ASP:HB2	1.96	0.45
1:B:275:ASP:N	1:B:275:ASP:OD1	2.45	0.45
2:A:273:PHE:CD1	2:A:273:PHE:O	2.70	0.45
1:B:1018:THR:HG21	1:B:1084:ILE:HD12	1.97	0.45
2:A:104:HIS:HA	2:A:108:GLN:OE1	2.17	0.45
2:A:129:VAL:HG11	2:A:155:TYR:CD1	2.51	0.45
1:B:88:LEU:HA	1:B:88:LEU:HD12	1.77	0.45
1:B:646:MET:SD	1:B:646:MET:N	2.90	0.45
2:A:154:VAL:HG23	2:A:206:LEU:HA	1.99	0.45
2:A:648:PHE:CG	2:A:651:ILE:HD11	2.52	0.45
1:B:1226:LYS:HG2	1:B:1232:THR:HG22	1.98	0.45
2:A:559:LEU:HD13	2:A:563:ILE:HD11	1.98	0.45
1:B:363:ALA:HB1	1:B:368:ASN:HB3	1.99	0.44
1:B:1199:GLN:O	1:B:1204:LYS:NZ	2.48	0.44
1:B:12:ASP:OD1	1:B:12:ASP:N	2.50	0.44
1:B:264:ARG:HD2	1:B:346:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:GLN:O	1:B:504:LEU:HD22	2.17	0.44
1:B:611:VAL:HG21	1:B:772:LYS:NZ	2.33	0.44
1:B:730:LYS:HB3	1:B:730:LYS:HE2	1.86	0.44
1:B:1205:ILE:HA	1:B:1262:VAL:HG12	1.99	0.44
2:A:164:ILE:HD13	2:A:164:ILE:HA	1.89	0.44
2:A:223:PHE:O	2:A:227:LEU:HD22	2.18	0.44
2:A:381:CYS:SG	2:A:622:GLN:HB3	2.57	0.44
1:B:36:PHE:CD1	1:B:36:PHE:N	2.86	0.44
1:B:130:ILE:HG22	1:B:132:THR:H	1.83	0.44
1:B:768:ASP:OD1	1:B:769:LEU:N	2.51	0.44
1:B:1241:ASP:OD1	1:B:1242:ASN:N	2.48	0.44
2:A:115:LEU:HB3	2:A:219:VAL:CG2	2.48	0.44
2:A:645:PHE:CZ	2:A:660:ALA:HB2	2.53	0.44
1:B:950:PRO:HG2	1:B:1065:ARG:NH1	2.33	0.44
1:B:605:GLY:O	1:B:609:GLN:HG3	2.17	0.43
1:B:648:TYR:HB2	1:B:651:ASP:HB2	2.00	0.43
1:B:657:ILE:O	1:B:893:ARG:NH2	2.51	0.43
2:A:157:GLY:O	2:A:210:ILE:HD13	2.18	0.43
1:B:755:THR:O	1:B:759:LYS:HE3	2.17	0.43
1:B:772:LYS:O	1:B:775:GLU:HG2	2.18	0.43
1:B:1057:LEU:HD11	1:B:1067:ILE:HG12	2.00	0.43
1:B:1121:LYS:HD3	1:B:1136:LEU:CB	2.46	0.43
1:B:1155:TYR:O	1:B:1156:ARG:HD2	2.18	0.43
2:A:536:PHE:CZ	2:A:540:LEU:HD12	2.53	0.43
1:B:36:PHE:CD2	1:B:88:LEU:HD21	2.53	0.43
1:B:98:ILE:O	1:B:104:GLY:HA3	2.19	0.43
1:B:541:LYS:HD2	1:B:541:LYS:HA	1.92	0.43
1:B:918:ASN:ND2	1:B:1062:ASP:O	2.52	0.43
2:A:455:VAL:HA	2:A:475:ASP:HB3	2.01	0.43
2:A:559:LEU:O	2:A:563:ILE:HD12	2.18	0.43
2:A:153:ILE:O	2:A:156:LEU:HB2	2.18	0.43
2:A:447:GLN:O	2:A:467:VAL:HA	2.19	0.43
1:B:1027:SER:HB3	1:B:1041:ILE:HD13	2.01	0.43
1:B:1037:ASP:OD1	1:B:1038:GLN:N	2.52	0.43
2:A:566:LEU:HD23	2:A:674:LEU:HB3	2.00	0.43
1:B:497:ASP:OD1	1:B:498:LEU:N	2.51	0.42
2:A:255:TRP:HB2	2:A:536:PHE:HD1	1.84	0.42
2:A:182:LEU:HD23	2:A:182:LEU:HA	1.85	0.42
2:A:193:SER:O	2:A:277:ARG:HG2	2.20	0.42
1:B:985:TRP:CD2	1:B:1019:ILE:HG21	2.54	0.42
2:A:156:LEU:O	2:A:159:MET:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:PHE:CD1	1:B:293:ILE:HD11	2.54	0.42
2:A:474:PHE:HD2	2:A:494:ILE:HG12	1.84	0.42
2:A:178:LEU:HB2	2:A:218:ILE:HG21	2.02	0.42
1:B:985:TRP:HB3	1:B:997:VAL:HG22	2.02	0.42
1:B:1143:VAL:HG12	1:B:1149:TYR:HE1	1.84	0.42
2:A:182:LEU:HD22	2:A:287:CYS:HB2	2.00	0.42
2:A:415:ILE:HD12	2:A:415:ILE:HA	1.83	0.42
2:A:109:TRP:HA	2:A:109:TRP:CE3	2.54	0.42
2:A:501:ASN:OD1	2:A:523:LYS:HG2	2.20	0.42
1:B:35:ALA:HB2	1:B:45:ILE:HG12	2.02	0.42
1:B:691:THR:O	1:B:695:ILE:HG12	2.20	0.42
1:B:709:VAL:HB	1:B:808:LEU:HD21	2.02	0.42
1:B:202:VAL:HG23	1:B:206:PRO:HA	2.01	0.42
1:B:716:ASN:OD1	1:B:720:LYS:HD2	2.20	0.42
2:A:181:SER:O	2:A:184:VAL:HG12	2.20	0.42
1:B:630:ILE:O	1:B:633:ILE:HG13	2.20	0.42
1:B:219:VAL:HG11	1:B:362:ASN:ND2	2.33	0.41
1:B:786:LYS:O	1:B:790:GLN:HG3	2.20	0.41
1:B:1153:SER:HB2	1:B:1293:GLU:OE2	2.19	0.41
1:B:626:LYS:H	1:B:626:LYS:HG2	1.41	0.41
1:B:1100:PHE:N	1:B:1284:PHE:O	2.47	0.41
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.93	0.41
1:B:1169:ASN:HB3	1:B:1171:ASP:OD1	2.20	0.41
2:A:285:LEU:O	2:A:289:VAL:HG23	2.21	0.41
1:B:1253:HIS:HB2	1:B:1262:VAL:HG21	2.01	0.41
2:A:530:LEU:HA	2:A:530:LEU:HD23	1.93	0.41
1:B:240:ASN:OD1	1:B:240:ASN:N	2.43	0.41
1:B:757:GLU:HA	1:B:760:ASN:HD21	1.85	0.41
2:A:216:LEU:HA	2:A:219:VAL:HG12	2.02	0.41
2:A:476:GLU:HA	2:A:496:SER:O	2.21	0.41
1:B:9:ASN:O	1:B:88:LEU:HD23	2.20	0.41
1:B:1154:LEU:HB3	1:B:1285:ILE:HD13	2.03	0.41
2:A:252:ALA:HB2	2:A:543:PHE:CE2	2.56	0.41
2:A:297:MET:N	2:A:297:MET:SD	2.93	0.41
2:A:392:ILE:O	2:A:396:VAL:HG23	2.19	0.41
2:A:445:GLU:OE1	2:A:445:GLU:N	2.54	0.41
2:A:598:LEU:O	2:A:602:THR:HG23	2.21	0.41
1:B:484:ASP:N	1:B:484:ASP:OD1	2.53	0.41
1:B:608:GLU:O	1:B:611:VAL:HG22	2.21	0.41
1:B:642:ASN:OD1	1:B:642:ASN:O	2.39	0.41
1:B:897:LYS:HE3	1:B:897:LYS:HB3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:984:ILE:HG12	1:B:998:VAL:HG12	2.03	0.41
1:B:995:GLN:OE1	1:B:995:GLN:HA	2.20	0.41
1:B:1127:ASN:O	1:B:1132:GLY:HA3	2.21	0.41
2:A:133:LEU:HB2	2:A:134:PRO:HD3	2.03	0.41
2:A:214:GLY:O	2:A:218:ILE:HG12	2.21	0.41
2:A:500:TYR:CE1	2:A:521:GLU:HB2	2.56	0.41
1:B:1110:PRO:HA	1:B:1161:ILE:HG22	2.03	0.41
1:B:1254:GLN:H	1:B:1254:GLN:HG3	1.69	0.41
2:A:208:SER:O	2:A:212:ILE:HG22	2.21	0.41
2:A:227:LEU:HD23	2:A:227:LEU:H	1.86	0.41
2:A:257:ILE:HG21	2:A:279:PHE:HB2	2.03	0.41
2:A:635:LYS:HA	2:A:635:LYS:HD3	1.59	0.41
1:B:563:LYS:O	1:B:563:LYS:NZ	2.39	0.40
1:B:706:TRP:HA	1:B:808:LEU:HD22	2.02	0.40
2:A:582:PHE:HD1	2:A:582:PHE:O	2.04	0.40
1:B:629:ASP:O	1:B:630:ILE:HD13	2.20	0.40
2:A:135:SER:HA	2:A:138:LYS:HE3	2.04	0.40
2:A:192:SER:HB3	2:A:204:CYS:HB3	2.03	0.40
2:A:236:LEU:HD23	2:A:236:LEU:HA	1.88	0.40
1:B:12:ASP:HB3	1:B:13:PRO:HD2	2.02	0.40
1:B:248:ASN:OD1	1:B:249:ALA:N	2.54	0.40
1:B:1148:ILE:HG22	1:B:1149:TYR:HD2	1.85	0.40
1:B:322:LEU:HD12	1:B:341:LEU:HB2	2.04	0.40
1:B:592:LYS:HD3	1:B:592:LYS:HA	1.92	0.40
1:B:905:ASN:HB3	1:B:915:GLN:HB3	2.04	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	B	1241/1329 (93%)	1193 (96%)	48 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	543/683 (80%)	518 (95%)	25 (5%)	0	100	100
All	All	1784/2012 (89%)	1711 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	B	1138/1204 (94%)	1106 (97%)	32 (3%)	38	59
2	A	459/580 (79%)	435 (95%)	24 (5%)	19	43
All	All	1597/1784 (90%)	1541 (96%)	56 (4%)	33	53

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	ASP
1	B	141	ASP
1	B	143	SER
1	B	144	TYR
1	B	165	CYS
1	B	197	GLU
1	B	280	ASN
1	B	301	LYS
1	B	326	ASP
1	B	344	MET
1	B	430	CYS
1	B	453	LEU
1	B	531	MET
1	B	537	PHE
1	B	614	PHE
1	B	621	VAL
1	B	625	ASP
1	B	626	LYS

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Mol	Chain	Res	Type
1	B	632	ILE
1	B	642	ASN
1	B	646	MET
1	B	767	ASP
1	B	824	TYR
1	B	884	GLU
1	B	893	ARG
1	B	934	TYR
1	B	971	ASN
1	B	1023	ARG
1	B	1025	ASN
1	B	1058	ASP
1	B	1135	TYR
1	B	1188	ASN
2	A	108	GLN
2	A	140	MET
2	A	150	LEU
2	A	155	TYR
2	A	196	GLN
2	A	222	TYR
2	A	224	SER
2	A	226	PHE
2	A	249	TYR
2	A	255	TRP
2	A	261	TYR
2	A	265	PHE
2	A	430	PHE
2	A	434	HIS
2	A	453	LYS
2	A	480	GLU
2	A	484	SER
2	A	528	MET
2	A	534	ASN
2	A	535	ASP
2	A	566	LEU
2	A	582	PHE
2	A	585	PHE
2	A	627	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	GLN
1	B	39	HIS
1	B	205	ASN
1	B	288	ASN
1	B	404	GLN
1	B	470	ASN
1	B	533	ASN
1	B	697	ASN
1	B	739	GLN
1	B	765	ASN
1	B	778	ASN
1	B	790	GLN
1	B	913	GLN
1	B	954	ASN
1	B	1026	ASN
1	B	1147	ASN
1	B	1199	GLN
1	B	1216	ASN
1	B	1233	ASN
2	A	434	HIS
2	A	446	ASN
2	A	447	GLN
2	A	516	ASN
2	A	553	ASN

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

8 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	$\#\|Z\| > 2$
3	NAG	C	1	2,3	14,14,15	0.39	0	17,19,21	0.61	0
3	FUC	C	2	3	10,10,11	0.44	0	14,14,16	0.39	0
4	NAG	D	1	4	14,14,15	1.65	2 (14%)	17,19,21	1.00	2 (11%)
4	NAG	D	2	4	14,14,15	0.38	0	17,19,21	0.74	0
4	BMA	D	3	4	11,11,12	0.41	0	15,15,17	1.05	1 (6%)
4	MAN	D	4	4	11,11,12	0.28	0	15,15,17	0.53	0
4	MAN	D	5	4	11,11,12	0.34	0	15,15,17	0.96	1 (6%)
4	FUC	D	6	4	10,10,11	0.85	1 (10%)	14,14,16	0.89	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
3	NAG	C	1	2,3	-	4/6/23/26	0/1/1/1
3	FUC	C	2	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	1/1/4/5	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	1/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	FUC	D	6	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C1-C2	4.71	1.59	1.52
4	D	1	NAG	O5-C1	-3.78	1.37	1.43
4	D	6	FUC	O5-C1	-2.03	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	5	MAN	C1-O5-C5	2.50	115.58	112.19
4	D	3	BMA	C1-C2-C3	2.34	112.54	109.67
4	D	1	NAG	C1-C2-N2	2.16	114.18	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	NAG	O3-C3-C2	2.05	113.70	109.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	FUC	C1
4	D	3	BMA	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
4	D	3	BMA	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7

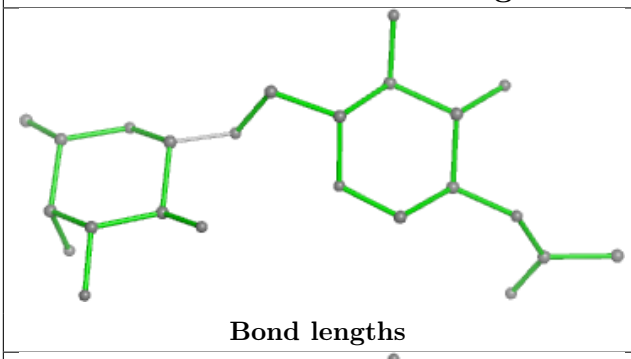
There are no ring outliers.

2 monomers are involved in 10 short contacts:

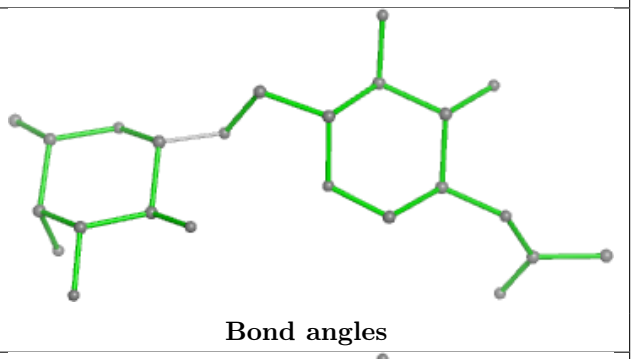
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	5	0
4	D	2	NAG	5	0

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

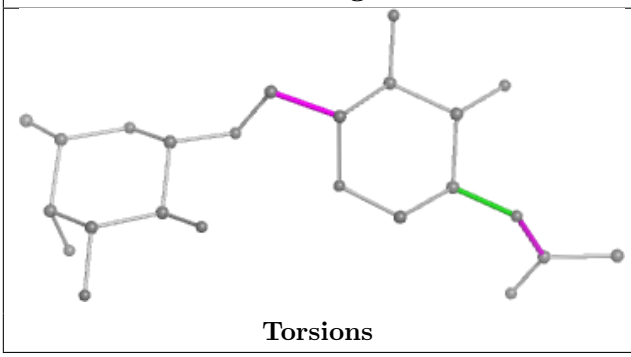
Oligosaccharide Chain C



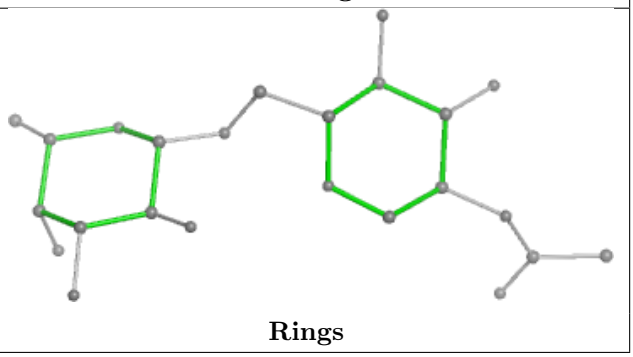
Bond lengths



Bond angles

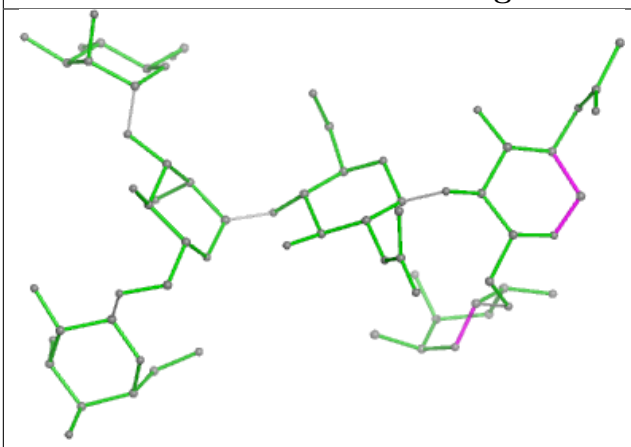


Torsions

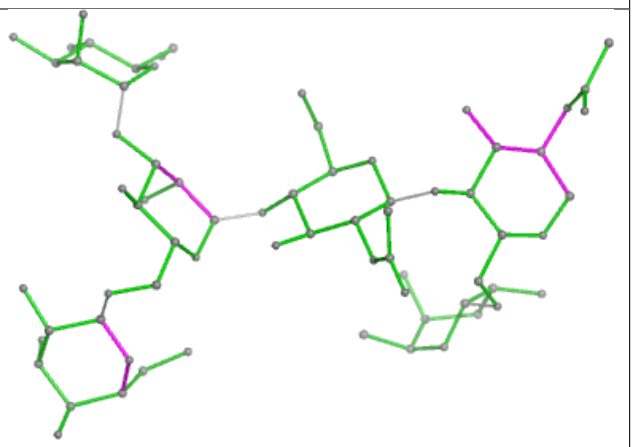


Rings

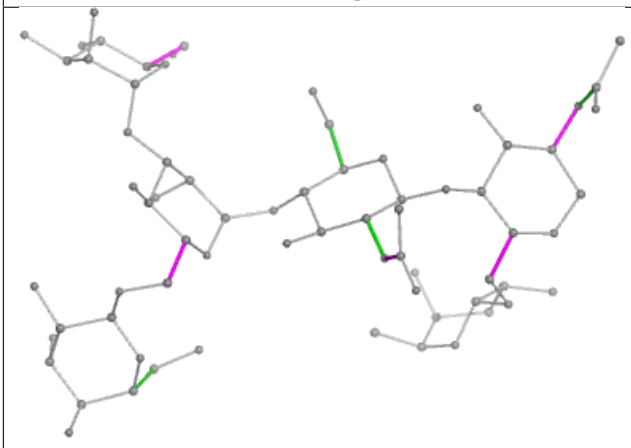
Oligosaccharide Chain D



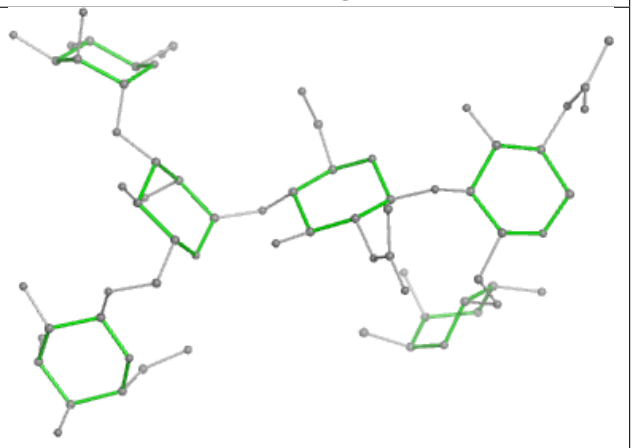
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

1 ligand is 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	A	701	2	14,14,15	0.25	0	17,19,21	0.36	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	A	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

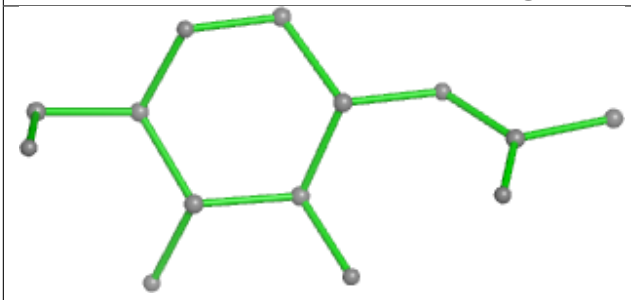
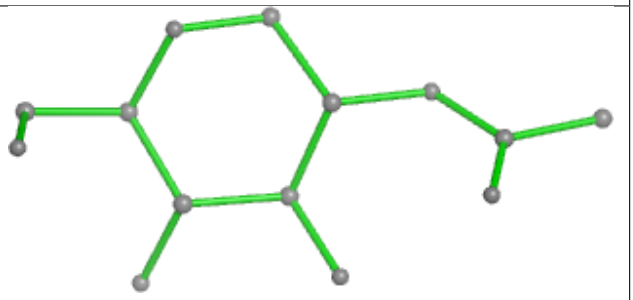
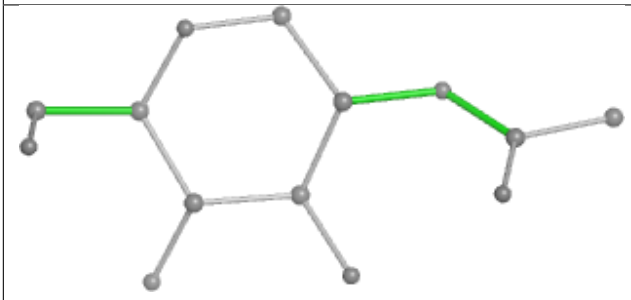
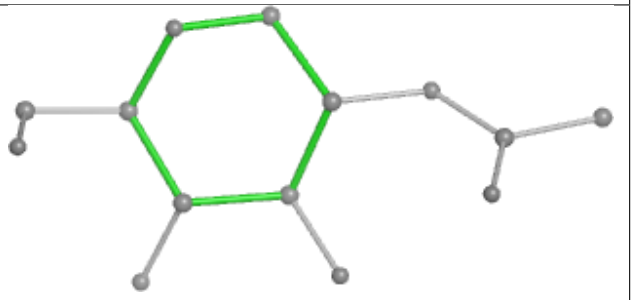
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 NAG A 701	
	
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.