



Full wwPDB EM Validation Report ⓘ

Sep 21, 2025 – 12:29 AM JST

PDB ID : 9UTC / pdb_00009utc
EMDB ID : EMD-64488
Title : The VFT domains of human sweet taste receptor TAS1R2 and TAS1R3 in the sucralose-bound state
Authors : Shi, Z.J.; Xu, W.X.; Yue, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2025-05-03
Resolution : 3.33 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

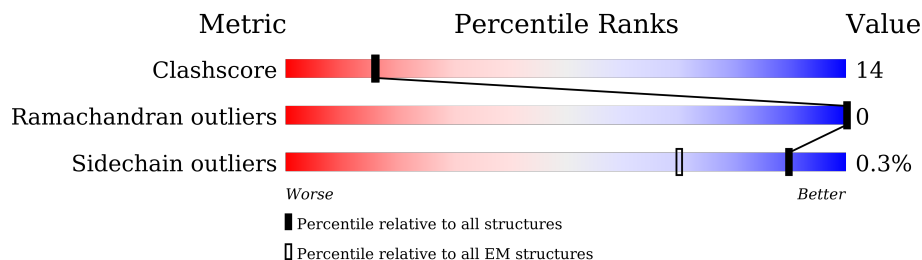
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1078	
2	B	1130	
3	C	2	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8143 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 Taste receptor type 1 member 2, Taste receptor type 1 member 2, Engineered red fluorescent protein mScarlet3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	500	Total	C	N	O	S	0	0
			4036	2581	677	752	26		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP Q8TE23
A	-2	LYS	-	expression tag	UNP Q8TE23
A	-1	THR	-	expression tag	UNP Q8TE23
A	0	ILE	-	expression tag	UNP Q8TE23
A	1	ILE	-	expression tag	UNP Q8TE23
A	2	ALA	-	expression tag	UNP Q8TE23
A	3	LEU	-	expression tag	UNP Q8TE23
A	4	SER	-	expression tag	UNP Q8TE23
A	5	TYR	-	expression tag	UNP Q8TE23
A	6	ILE	-	expression tag	UNP Q8TE23
A	7	PHE	-	expression tag	UNP Q8TE23
A	8	CYS	-	expression tag	UNP Q8TE23
A	9	LEU	-	expression tag	UNP Q8TE23
A	10	VAL	-	expression tag	UNP Q8TE23
A	11	PHE	-	expression tag	UNP Q8TE23
A	12	ALA	-	expression tag	UNP Q8TE23
A	13	GLY	-	expression tag	UNP Q8TE23
A	14	SER	-	expression tag	UNP Q8TE23
A	15	ASP	-	expression tag	UNP Q8TE23
A	16	TYR	-	expression tag	UNP Q8TE23
A	17	LYS	-	expression tag	UNP Q8TE23
A	18	ASP	-	expression tag	UNP Q8TE23
A	19	ASP	-	expression tag	UNP Q8TE23
A	20	ASP	-	expression tag	UNP Q8TE23
A	21	ASP	-	expression tag	UNP Q8TE23
A	22	LYS	-	expression tag	UNP Q8TE23
A	23	GLY	-	expression tag	UNP Q8TE23

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q8TE23
A	25	ALA	-	expression tag	UNP Q8TE23

- Molecule 2 is a protein called Taste receptor type 1 member 3,mNeonGreen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4084	2577	722	752	33		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q7RTX0
B	-6	LYS	-	expression tag	UNP Q7RTX0
B	-5	THR	-	expression tag	UNP Q7RTX0
B	-4	ILE	-	expression tag	UNP Q7RTX0
B	-3	ILE	-	expression tag	UNP Q7RTX0
B	-2	ALA	-	expression tag	UNP Q7RTX0
B	-1	LEU	-	expression tag	UNP Q7RTX0
B	0	SER	-	expression tag	UNP Q7RTX0
B	1	TYR	-	expression tag	UNP Q7RTX0
B	2	ILE	-	expression tag	UNP Q7RTX0
B	3	PHE	-	expression tag	UNP Q7RTX0
B	4	CYS	-	expression tag	UNP Q7RTX0
B	5	LEU	-	expression tag	UNP Q7RTX0
B	6	VAL	-	expression tag	UNP Q7RTX0
B	7	PHE	-	expression tag	UNP Q7RTX0
B	8	ALA	-	expression tag	UNP Q7RTX0
B	9	GLY	-	expression tag	UNP Q7RTX0
B	10	SER	-	expression tag	UNP Q7RTX0
B	11	ASP	-	expression tag	UNP Q7RTX0
B	12	TYR	-	expression tag	UNP Q7RTX0
B	13	LYS	-	expression tag	UNP Q7RTX0
B	14	ASP	-	expression tag	UNP Q7RTX0
B	15	ASP	-	expression tag	UNP Q7RTX0
B	16	ASP	-	expression tag	UNP Q7RTX0
B	17	ASP	-	expression tag	UNP Q7RTX0
B	18	LYS	-	expression tag	UNP Q7RTX0
B	19	GLY	-	expression tag	UNP Q7RTX0
B	20	SER	-	expression tag	UNP Q7RTX0
B	853	GLY	-	linker	UNP Q7RTX0
B	854	SER	-	linker	UNP Q7RTX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	855	SER	-	linker	UNP Q7RTX0
B	856	GLY	-	linker	UNP Q7RTX0
B	857	LEU	-	linker	UNP Q7RTX0
B	858	GLU	-	linker	UNP Q7RTX0
B	859	VAL	-	linker	UNP Q7RTX0
B	860	LEU	-	linker	UNP Q7RTX0
B	861	PHE	-	linker	UNP Q7RTX0
B	862	GLN	-	linker	UNP Q7RTX0
B	863	GLY	-	linker	UNP Q7RTX0
B	864	PRO	-	linker	UNP Q7RTX0
B	865	SER	-	linker	UNP Q7RTX0
B	866	GLY	-	linker	UNP Q7RTX0
B	867	GLY	-	linker	UNP Q7RTX0
B	1103	GLY	-	expression tag	UNP A0A1S4NYF2
B	1104	SER	-	expression tag	UNP A0A1S4NYF2
B	1105	GLU	-	expression tag	UNP A0A1S4NYF2
B	1106	ASN	-	expression tag	UNP A0A1S4NYF2
B	1107	LEU	-	expression tag	UNP A0A1S4NYF2
B	1108	TYR	-	expression tag	UNP A0A1S4NYF2
B	1109	PHE	-	expression tag	UNP A0A1S4NYF2
B	1110	GLN	-	expression tag	UNP A0A1S4NYF2
B	1111	SER	-	expression tag	UNP A0A1S4NYF2
B	1112	SER	-	expression tag	UNP A0A1S4NYF2
B	1113	GLY	-	expression tag	UNP A0A1S4NYF2
B	1114	HIS	-	expression tag	UNP A0A1S4NYF2
B	1115	HIS	-	expression tag	UNP A0A1S4NYF2
B	1116	HIS	-	expression tag	UNP A0A1S4NYF2
B	1117	HIS	-	expression tag	UNP A0A1S4NYF2
B	1118	HIS	-	expression tag	UNP A0A1S4NYF2
B	1119	HIS	-	expression tag	UNP A0A1S4NYF2
B	1120	HIS	-	expression tag	UNP A0A1S4NYF2
B	1121	HIS	-	expression tag	UNP A0A1S4NYF2
B	1122	HIS	-	expression tag	UNP A0A1S4NYF2

- Molecule 3 is an oligosaccharide called 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	Cl	O	0	0
			23	12	3	8		

[illegible]

- Molecule 2: Taste receptor type 1 member 3,mNeonGreen

Chain B: 34% 12% 53%

[illegible]

- Molecule 3: 4-chloro-4-deoxy- α -D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy- β -D-fructofuranose

Chain C:  50% 50%

REV 1
REL 2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: RRJ, RRY

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	0.21	0/4137	0.38	0/5637
2	B	0.20	0/4183	0.36	0/5676
All	All	0.21	0/8320	0.37	0/11313

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4036	0	3903	124	0
2	B	4084	0	3969	107	0
3	C	23	0	0	1	0
All	All	8143	0	7872	228	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 14.

All (228) 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:439:ASP:OD1	1:A:440:PRO:CD	1.71	1.36
1:A:402:LEU:HD13	1:A:423:GLU:CG	1.73	1.18
1:A:249:MET:SD	1:A:283:HIS:HD2	1.69	1.14
2:B:509:ARG:HD2	2:B:519:TYR:CE2	1.83	1.12
2:B:509:ARG:HD2	2:B:519:TYR:CZ	1.89	1.07
1:A:402:LEU:CD1	1:A:423:GLU:HG3	1.91	0.99
1:A:439:ASP:OD1	1:A:440:PRO:HD2	0.80	0.97
2:B:509:ARG:CD	2:B:519:TYR:CZ	2.47	0.96
1:A:249:MET:SD	1:A:283:HIS:CD2	2.59	0.94
1:A:402:LEU:HD13	1:A:423:GLU:HG3	0.95	0.93
1:A:302:GLU:OE2	3:C:2:RRJ:O2	1.94	0.86
1:A:439:ASP:CG	1:A:440:PRO:HD2	1.99	0.82
2:B:509:ARG:HD3	2:B:519:TYR:CZ	2.21	0.75
2:B:507:GLN:O	2:B:530:ARG:NH1	2.19	0.75
2:B:54:ARG:NH2	2:B:58:SER:O	2.21	0.74
1:A:172:ARG:O	1:A:441:GLN:OE1	2.07	0.73
2:B:181:PRO:O	2:B:431:TYR:OH	2.04	0.73
1:A:521:LEU:O	1:A:524:THR:OG1	2.05	0.70
2:B:509:ARG:CD	2:B:519:TYR:CE2	2.70	0.70
1:A:248:ASN:OD1	1:A:248:ASN:O	2.10	0.69
1:A:274:VAL:HG11	1:A:281:LEU:HD11	1.75	0.69
2:B:331:LEU:O	2:B:331:LEU:HD23	1.94	0.68
1:A:211:SER:OG	1:A:213:ASP:OD1	2.12	0.68
1:A:321:THR:HG21	1:A:483:TRP:CE3	2.29	0.67
1:A:289:LEU:HB2	1:A:319:LEU:HD11	1.76	0.66
2:B:347:ASP:OD1	2:B:350:PHE:N	2.28	0.66
1:A:321:THR:HG21	1:A:483:TRP:CZ3	2.32	0.65
1:A:287:GLU:OE2	1:A:287:GLU:N	2.30	0.64
2:B:491:ASP:OD1	2:B:491:ASP:O	2.16	0.64
2:B:122:SER:OG	2:B:124:ASP:OD1	2.10	0.64
2:B:529:TYR:N	2:B:539:THR:O	2.31	0.63
1:A:136:VAL:HG22	1:A:420:LEU:HD12	1.80	0.62
1:A:188:ASP:OD1	1:A:189:HIS:N	2.33	0.62
1:A:402:LEU:CD1	1:A:423:GLU:CG	2.66	0.61
1:A:194:MET:O	1:A:198:MET:HG3	2.01	0.61
1:A:76:ARG:HA	1:A:76:ARG:CZ	2.31	0.61
2:B:419:ASP:OD1	2:B:419:ASP:N	2.33	0.61
2:B:317:GLN:OE1	2:B:317:GLN:N	2.34	0.60
1:A:76:ARG:HA	1:A:76:ARG:NH1	2.17	0.59
2:B:126:ALA:O	2:B:134:TYR:OH	2.20	0.59
2:B:370:CYS:SG	2:B:373:CYS:N	2.72	0.59
2:B:426:LEU:O	2:B:430:MET:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:HA	1:A:444:VAL:HG22	1.85	0.59
2:B:457:LYS:HE2	2:B:457:LYS:HA	1.85	0.58
1:A:29:LEU:HB2	1:A:96:TYR:CE1	2.39	0.58
1:A:300:ALA:N	1:A:323:LEU:O	2.33	0.58
1:A:376:ILE:HD11	1:A:457:ARG:NH1	2.19	0.57
2:B:509:ARG:HD2	2:B:519:TYR:CD2	2.37	0.57
2:B:223:LEU:HD12	2:B:242:LEU:CD2	2.34	0.57
1:A:326:THR:O	1:A:449:GLU:N	2.33	0.57
1:A:281:LEU:HD12	1:A:285:PHE:CE2	2.40	0.57
1:A:151:ALA:HB2	1:A:180:LEU:HD13	1.86	0.56
1:A:252:GLU:OE2	1:A:252:GLU:N	2.27	0.56
1:A:363:CYS:SG	1:A:364:ASP:N	2.79	0.56
2:B:245:LEU:HD23	2:B:245:LEU:H	1.69	0.56
2:B:215:ASP:HA	2:B:242:LEU:HD13	1.88	0.55
2:B:172:GLU:HB3	2:B:225:ILE:HD11	1.87	0.55
2:B:199:GLU:O	2:B:203:GLU:HG2	2.06	0.55
1:A:81:GLU:OE2	1:A:389:TYR:OH	2.23	0.55
1:A:123:PRO:HB2	1:A:125:GLN:HE22	1.72	0.55
1:A:183:THR:HG21	1:A:391:ALA:HB2	1.88	0.54
2:B:456:LEU:N	2:B:472:GLY:O	2.39	0.54
1:A:376:ILE:HD11	1:A:457:ARG:CZ	2.37	0.54
2:B:505:GLU:OE2	2:B:530:ARG:NH2	2.41	0.54
1:A:71:LEU:HD21	1:A:384:VAL:HG23	1.88	0.54
1:A:360:ASN:O	1:A:360:ASN:ND2	2.41	0.54
1:A:384:VAL:O	1:A:387:SER:OG	2.24	0.54
2:B:148:GLU:HA	2:B:148:GLU:OE1	2.08	0.53
2:B:217:GLU:OE1	2:B:218:TYR:N	2.41	0.53
1:A:433:ASP:O	1:A:434:HIS:ND1	2.40	0.53
1:A:41:LEU:HD21	1:A:72:MET:HE1	1.91	0.53
2:B:518:CYS:SG	2:B:519:TYR:N	2.80	0.53
1:A:82:ILE:HG12	1:A:88:LEU:HD23	1.91	0.53
1:A:278:ASP:OD1	1:A:279:LEU:N	2.42	0.53
1:A:465:VAL:HG11	1:A:481:ILE:HD12	1.89	0.52
2:B:404:LEU:HA	2:B:407:THR:HG22	1.90	0.52
1:A:138:VAL:H	1:A:159:LEU:HD21	1.74	0.52
2:B:327:ARG:NH2	2:B:455:ASP:OD2	2.42	0.52
1:A:139:ILE:HD13	1:A:392:VAL:HG22	1.91	0.52
2:B:151:MET:HE1	2:B:173:LEU:HB3	1.90	0.52
2:B:534:ASP:OD1	2:B:534:ASP:N	2.43	0.52
1:A:205:TRP:O	1:A:493:SER:OG	2.28	0.52
1:A:452:GLN:OE1	1:A:453:TRP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TYR:HE2	2:B:93:LEU:HD21	1.75	0.52
2:B:161:LEU:HB3	2:B:427:LEU:HD22	1.92	0.51
1:A:316:LEU:HA	1:A:319:LEU:HD13	1.92	0.51
2:B:83:ILE:CD1	2:B:95:LEU:HD12	2.40	0.51
1:A:79:VAL:HA	1:A:82:ILE:HD12	1.93	0.51
2:B:320:THR:HG21	2:B:487:TRP:CE3	2.46	0.51
1:A:141:PRO:HB2	1:A:147:VAL:HG22	1.93	0.51
2:B:546:TRP:N	2:B:555:PHE:O	2.42	0.51
2:B:445:ASP:C	2:B:445:ASP:OD1	2.55	0.50
1:A:257:LEU:HD22	1:A:287:GLU:OE1	2.11	0.50
1:A:439:ASP:OD1	1:A:440:PRO:N	2.41	0.50
1:A:147:VAL:HG21	1:A:166:ALA:HB2	1.94	0.50
1:A:321:THR:O	1:A:321:THR:HG23	2.11	0.50
2:B:223:LEU:HD12	2:B:242:LEU:HD21	1.92	0.50
1:A:27:PHE:CD2	1:A:361:GLN:O	2.65	0.49
2:B:509:ARG:HD3	2:B:519:TYR:OH	2.12	0.49
1:A:242:THR:O	1:A:243:LEU:HD22	2.12	0.49
1:A:376:ILE:HD11	1:A:457:ARG:NH2	2.28	0.49
1:A:421:LEU:HA	1:A:424:ILE:HG22	1.93	0.49
2:B:509:ARG:CD	2:B:519:TYR:CE1	2.95	0.49
1:A:361:GLN:O	1:A:362:GLU:HG2	2.13	0.48
1:A:531:ASP:C	1:A:531:ASP:OD1	2.56	0.48
2:B:209:VAL:HG23	2:B:270:VAL:HG23	1.96	0.48
1:A:282:TYR:HE1	1:A:313:LEU:HD13	1.79	0.48
2:B:287:SER:CB	2:B:318:MET:HE1	2.44	0.48
2:B:124:ASP:OD1	2:B:124:ASP:N	2.37	0.48
2:B:172:GLU:OE1	2:B:172:GLU:HA	2.13	0.48
1:A:119:ASP:N	1:A:119:ASP:OD1	2.40	0.48
1:A:162:ILE:HD13	1:A:395:VAL:CG2	2.44	0.48
2:B:139:LEU:HD13	2:B:426:LEU:HD11	1.96	0.48
2:B:488:HIS:CD2	2:B:489:THR:HG23	2.49	0.48
2:B:344:LEU:HD11	2:B:350:PHE:CD1	2.49	0.47
1:A:172:ARG:HG2	1:A:443:ASP:OD2	2.13	0.47
1:A:361:GLN:O	1:A:361:GLN:HG3	2.14	0.47
1:A:527:ASN:ND2	1:A:530:GLU:OE1	2.48	0.47
2:B:150:ALA:HB1	2:B:183:PHE:CZ	2.49	0.47
1:A:159:LEU:C	1:A:159:LEU:HD23	2.39	0.47
2:B:505:GLU:O	2:B:530:ARG:NH2	2.44	0.47
2:B:212:LEU:HB3	2:B:273:LEU:HD12	1.96	0.47
2:B:256:VAL:O	2:B:260:LEU:HD22	2.13	0.47
2:B:196:ALA:HB1	2:B:324:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:THR:O	2:B:305:THR:OG1	2.26	0.47
1:A:294:THR:OG1	1:A:295:GLY:N	2.48	0.46
2:B:249:ASP:O	2:B:252:ARG:N	2.44	0.46
1:A:27:PHE:CE1	1:A:72:MET:SD	3.09	0.46
1:A:70:ASN:ND2	1:A:377:LEU:HD22	2.32	0.45
1:A:124:ILE:HB	2:B:115:MET:HE3	1.98	0.45
2:B:435:PHE:HD2	2:B:437:VAL:HG23	1.82	0.45
1:A:215:TYR:O	1:A:219:ASN:ND2	2.49	0.45
1:A:255:GLN:OE1	1:A:255:GLN:C	2.59	0.45
1:A:333:PRO:HD3	1:A:432:LEU:HD11	1.98	0.45
2:B:115:MET:HE2	2:B:115:MET:HA	1.97	0.45
2:B:167:TYR:O	2:B:187:VAL:HG21	2.17	0.45
2:B:194:LEU:HD21	2:B:274:PHE:CD1	2.52	0.45
1:A:172:ARG:NH1	1:A:443:ASP:OD2	2.49	0.45
1:A:257:LEU:O	1:A:261:VAL:HG22	2.17	0.45
2:B:434:THR:HG23	2:B:434:THR:O	2.16	0.45
2:B:111:LYS:N	2:B:112:PRO:HD2	2.32	0.45
1:A:204:ASN:OD1	1:A:204:ASN:C	2.60	0.45
1:A:221:GLN:HE22	2:B:242:LEU:HD12	1.80	0.45
1:A:464:SER:O	1:A:479:GLN:NE2	2.50	0.45
1:A:450:ILE:HB	1:A:466:ALA:HB3	1.99	0.45
2:B:230:ALA:HB1	2:B:235:ILE:O	2.17	0.45
2:B:166:SER:OG	2:B:167:TYR:N	2.49	0.44
2:B:76:MET:HE2	2:B:99:LEU:HD22	1.99	0.44
1:A:293:PHE:CZ	1:A:296:ALA:HB2	2.53	0.44
2:B:79:ALA:O	2:B:83:ILE:HG12	2.17	0.44
2:B:171:MET:HE3	2:B:221:GLN:HG3	1.98	0.44
1:A:261:VAL:HG12	1:A:288:VAL:HG22	1.98	0.44
1:A:531:ASP:OD1	1:A:531:ASP:O	2.36	0.44
1:A:109:GLN:C	1:A:109:GLN:CD	2.86	0.44
1:A:96:TYR:HD2	1:A:98:ILE:HG12	1.82	0.44
1:A:174:LYS:HD2	1:A:174:LYS:N	2.32	0.44
1:A:281:LEU:O	1:A:282:TYR:C	2.61	0.44
1:A:524:THR:HA	1:A:537:ALA:HA	2.00	0.44
2:B:535:ASP:OD1	2:B:535:ASP:N	2.51	0.44
1:A:76:ARG:CZ	1:A:96:TYR:CE1	3.01	0.44
2:B:97:TYR:CD1	2:B:97:TYR:N	2.84	0.44
1:A:88:LEU:O	1:A:400:HIS:CD2	2.71	0.43
1:A:169:ASP:OD1	1:A:172:ARG:HD3	2.19	0.43
2:B:342:LEU:O	2:B:346:THR:HG23	2.18	0.43
1:A:520:CYS:SG	1:A:524:THR:OG1	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:HD2	1:A:361:GLN:O	2.02	0.43
1:A:477:ASN:OD1	1:A:477:ASN:O	2.36	0.43
1:A:91:GLY:O	1:A:92:VAL:C	2.61	0.43
1:A:281:LEU:HD12	1:A:285:PHE:CD2	2.54	0.43
2:B:223:LEU:HD12	2:B:242:LEU:HD23	2.00	0.43
2:B:470:ASP:OD1	2:B:470:ASP:C	2.62	0.43
2:B:165:VAL:HG23	2:B:184:PHE:O	2.18	0.43
2:B:400:VAL:HG22	2:B:430:MET:HE1	2.00	0.43
2:B:545:GLU:HA	2:B:556:ARG:HA	2.00	0.43
2:B:299:ALA:HB3	2:B:304:LEU:HD13	2.01	0.43
1:A:28:TYR:CD1	1:A:29:LEU:N	2.87	0.43
2:B:80:VAL:O	2:B:83:ILE:HG13	2.19	0.43
2:B:151:MET:HE2	2:B:171:MET:HE2	2.00	0.42
2:B:326:GLN:NE2	2:B:452:MET:SD	2.87	0.42
2:B:528:SER:HA	2:B:540:PHE:HA	2.01	0.42
2:B:70:LEU:O	2:B:74:LEU:HG	2.19	0.42
2:B:307:ASP:O	2:B:307:ASP:OD1	2.37	0.42
2:B:59:SER:HG	2:B:107:VAL:C	2.27	0.42
1:A:127:ASP:OD1	1:A:127:ASP:C	2.63	0.42
1:A:159:LEU:HA	1:A:417:PRO:HB2	2.01	0.42
2:B:76:MET:HE2	2:B:99:LEU:CD2	2.49	0.42
2:B:274:PHE:HA	2:B:300:SER:OG	2.19	0.42
1:A:498:ARG:NH1	1:A:499:CYS:O	2.53	0.42
2:B:65:PHE:CZ	2:B:67:SER:HA	2.55	0.42
2:B:249:ASP:HA	2:B:252:ARG:HB2	2.02	0.42
2:B:83:ILE:HD12	2:B:95:LEU:HD12	2.01	0.42
2:B:131:TYR:CD1	2:B:131:TYR:C	2.97	0.42
1:A:147:VAL:HG13	1:A:180:LEU:HD11	2.02	0.42
1:A:109:GLN:N	1:A:110:PRO:CD	2.83	0.41
1:A:173:ASP:OD1	1:A:175:VAL:HG12	2.20	0.41
2:B:549:GLU:O	2:B:550:ARG:HG2	2.20	0.41
1:A:138:VAL:HG21	1:A:154:LEU:HD11	2.03	0.41
1:A:194:MET:HE2	1:A:325:ILE:CD1	2.50	0.41
1:A:510:ILE:HD13	2:B:265:GLN:NE2	2.35	0.41
1:A:463:GLN:OE1	1:A:464:SER:N	2.53	0.41
1:A:276:SER:HB2	1:A:281:LEU:CD2	2.50	0.41
1:A:402:LEU:HD21	1:A:419:GLN:HB3	2.03	0.41
2:B:91:PRO:HG3	2:B:411:ASN:O	2.21	0.41
2:B:331:LEU:HD23	2:B:334:PHE:HB2	2.02	0.41
2:B:207:ASN:OD1	2:B:207:ASN:N	2.53	0.41
1:A:33:TYR:O	1:A:94:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:N	1:A:364:ASP:OD1	2.45	0.41
1:A:504:LYS:N	1:A:518:ILE:O	2.52	0.41
2:B:93:LEU:HD12	2:B:93:LEU:HA	1.99	0.41
2:B:108:VAL:HG22	2:B:108:VAL:O	2.21	0.41
2:B:377:THR:OG1	2:B:378:LEU:N	2.53	0.41
1:A:82:ILE:HG13	1:A:393:TYR:CE1	2.56	0.40
2:B:487:TRP:O	2:B:488:HIS:ND1	2.54	0.40
2:B:140:ALA:HB3	2:B:400:VAL:HG11	2.02	0.40
2:B:304:LEU:HD21	2:B:457:LYS:HB2	2.02	0.40
2:B:387:HIS:O	2:B:390:THR:HG22	2.21	0.40
2:B:426:LEU:O	2:B:427:LEU:C	2.64	0.40
1:A:166:ALA:HB1	1:A:171:LEU:CD1	2.51	0.40
1:A:302:GLU:HA	1:A:325:ILE:O	2.21	0.40
1:A:308:PRO:HB3	1:A:376:ILE:HG21	2.02	0.40
1:A:58:MET:SD	1:A:58:MET:N	2.94	0.40
1:A:283:HIS:O	1:A:287:GLU:OE2	2.39	0.40
2:B:26:SER:HB3	2:B:369:ARG:HA	2.03	0.40
1:A:167:ILE:HD13	1:A:167:ILE:HA	1.93	0.40
1:A:182:ARG:HB3	1:A:443:ASP:OD1	2.21	0.40
1:A:192:GLU:CD	1:A:473:ARG:HE	2.29	0.40
1:A:225:GLU:CD	1:A:225:GLU:C	2.89	0.40
2:B:98:ASP:O	2:B:100:PHE:HD1	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	A	494/1078 (46%)	451 (91%)	43 (9%)	0	100	100
2	B	522/1130 (46%)	470 (90%)	52 (10%)	0	100	100
All	All	1016/2208 (46%)	921 (91%)	95 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/955 (48%)	453 (100%)	2 (0%)	89	93
2	B	442/941 (47%)	441 (100%)	1 (0%)	92	95
All	All	897/1896 (47%)	894 (100%)	3 (0%)	90	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	SER
1	A	393	TYR
2	B	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	120	ASN
1	A	125	GLN
1	A	248	ASN
1	A	283	HIS
1	A	441	GLN
1	A	541	ASN
2	B	341	HIS
2	B	462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	RRY	C	1	3	10,12,12	0.72	0	8,18,18	0.64	0
3	RRJ	C	2	3	10,11,12	1.20	1 (10%)	11,15,17	1.14	1 (9%)

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	RRY	C	1	3	-	0/5/24/24	0/1/1/1
3	RRJ	C	2	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	RRJ	C4-C5	2.59	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	RRJ	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

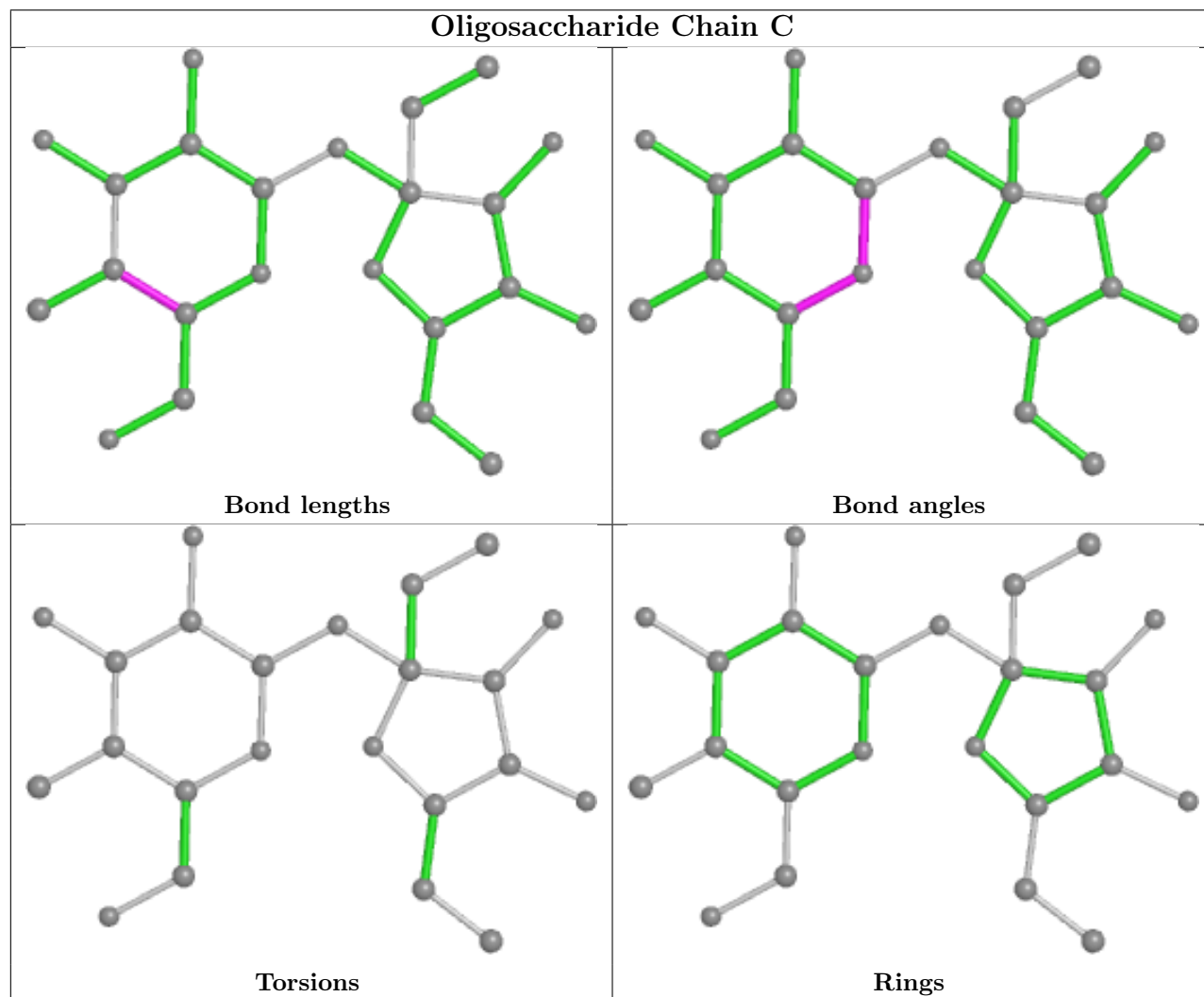
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	RRJ	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.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.