



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 AM UTC

PDB ID : 1MG1 / pdb_00001mg1
Title : HTLV-1 GP21 ECTODOMAIN / MALTOSE-BINDING PROTEIN CHIMERA
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Deposited on : 1999-03-01
Resolution : 2.50 Å (reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

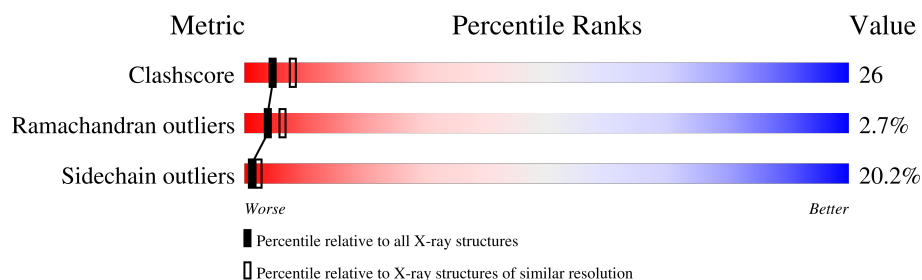
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

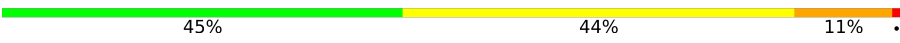
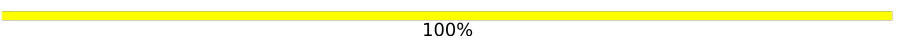
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	450	 45% 44% 11% .
2	B	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3545 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PROTEIN (HTLV-1 GP21 ECTODOMAIN/MALTOSE-BINDING PROTEIN CHIMERA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3483	2232	580	661	10			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

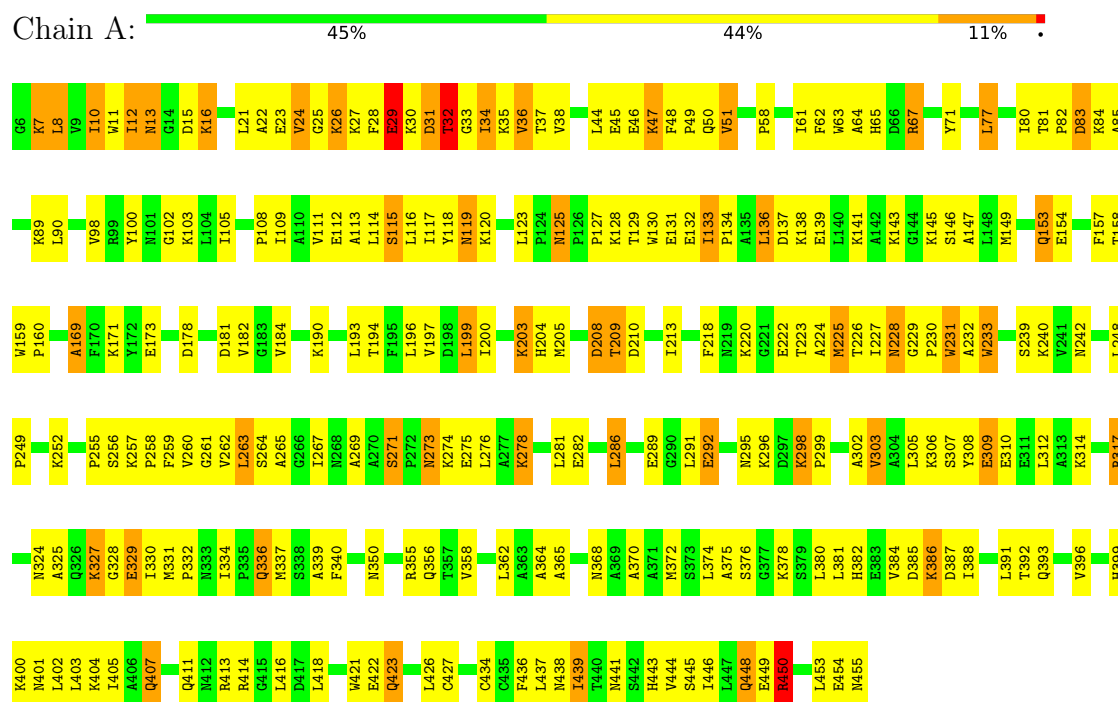
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (HTLV-1 GP21 ECTODOMAIN/MALTOSE-BINDING PROTEIN CHIMERA)



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	102.95Å 102.95Å 118.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	94.6 (40.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.223 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3545	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, CL

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	0.40	0/3562	0.93	11/4833 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	N-CA-C	-7.25	104.56	113.41
1	A	312	LEU	N-CA-C	-6.49	106.00	114.04
1	A	374	LEU	N-CA-C	-6.20	104.58	111.71
1	A	436	PHE	N-CA-C	6.02	118.48	108.13
1	A	154	GLU	CA-C-N	5.85	126.26	119.47
1	A	154	GLU	C-N-CA	5.85	126.26	119.47
1	A	271	SER	N-CA-C	5.27	116.30	109.65
1	A	208	ASP	N-CA-C	-5.27	106.83	113.20
1	A	386	LYS	N-CA-C	-5.23	105.06	111.75
1	A	133	ILE	CB-CA-C	-5.13	108.91	114.35
1	A	34	ILE	N-CA-C	5.00	115.44	108.84

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	3483	0	3464	181	0
2	B	23	0	21	0	0
3	A	2	0	0	0	0
4	A	37	0	0	5	0
All	All	3545	0	3485	181	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 26.

All (181) 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:334:ILE:HB	1:A:336:GLN:HE22	1.37	0.90
1:A:334:ILE:HB	1:A:336:GLN:NE2	1.92	0.84
1:A:116:LEU:HD22	1:A:249:PRO:HD3	1.61	0.80
1:A:260:VAL:HG13	1:A:330:ILE:HD12	1.66	0.77
1:A:445:SER:HA	1:A:448:GLN:HG3	1.65	0.77
1:A:317:ARG:HH11	1:A:317:ARG:HG3	1.50	0.76
1:A:29:GLU:O	1:A:33:GLY:N	2.18	0.75
1:A:10:ILE:HG21	1:A:21:LEU:HD21	1.71	0.73
1:A:98:VAL:HG21	1:A:108:PRO:HD3	1.71	0.72
1:A:278:LYS:O	1:A:282:GLU:HB2	1.89	0.71
1:A:380:LEU:O	1:A:384:VAL:HG23	1.91	0.70
1:A:190:LYS:O	1:A:194:THR:HG23	1.92	0.69
1:A:90:LEU:HD23	1:A:108:PRO:HG2	1.74	0.69
1:A:32:THR:HG22	1:A:34:ILE:H	1.57	0.69
1:A:332:PRO:HG2	1:A:337:MET:SD	2.33	0.68
1:A:382:HIS:HB2	4:A:475:HOH:O	1.93	0.68
1:A:372:MET:HE3	1:A:376:SER:HB2	1.74	0.68
1:A:350:ASN:HB3	1:A:356:GLN:HB2	1.77	0.67
1:A:256:SER:O	1:A:258:PRO:HD3	1.95	0.66
1:A:384:VAL:O	1:A:388:ILE:HG13	1.96	0.66
1:A:273:ASN:HB3	1:A:276:LEU:HD22	1.77	0.65
1:A:260:VAL:HG12	1:A:329:GLU:O	1.97	0.65
1:A:100:TYR:HB3	1:A:105:ILE:HD13	1.79	0.65
1:A:28:PHE:O	1:A:32:THR:HB	1.97	0.65
1:A:399:HIS:O	1:A:402:LEU:HB2	1.98	0.64
1:A:8:LEU:HD23	1:A:36:VAL:CG2	2.28	0.64
1:A:153:GLN:NE2	1:A:209:THR:O	2.31	0.63
1:A:255:PRO:HB3	4:A:488:HOH:O	1.97	0.63
1:A:239:SER:O	1:A:240:LYS:HG2	1.99	0.63
1:A:317:ARG:HG3	1:A:317:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LEU:HD13	1:A:426:LEU:HD13	1.81	0.62
1:A:454:GLU:O	1:A:454:GLU:HG2	2.00	0.62
1:A:117:ILE:HB	1:A:226:THR:CG2	2.30	0.61
1:A:112:GLU:O	1:A:260:VAL:HG23	2.00	0.61
1:A:401:ASN:O	1:A:405:ILE:HG13	2.00	0.61
1:A:157:PHE:O	1:A:160:PRO:HD2	2.00	0.61
1:A:46:GLU:O	1:A:50:GLN:HG3	2.00	0.61
1:A:45:GLU:HB2	1:A:67:ARG:CD	2.33	0.59
1:A:123:LEU:HD21	1:A:127:PRO:HD3	1.85	0.59
1:A:67:ARG:HD3	1:A:71:TYR:OH	2.03	0.58
1:A:184:VAL:O	1:A:362:LEU:HD22	2.04	0.58
1:A:411:GLN:O	1:A:414:ARG:HB2	2.03	0.57
1:A:80:ILE:HG22	1:A:267:ILE:HD13	1.87	0.57
1:A:292:GLU:HG3	1:A:308:TYR:CZ	2.39	0.57
1:A:273:ASN:N	1:A:273:ASN:OD1	2.37	0.57
1:A:65:HIS:CD2	1:A:262:VAL:H	2.23	0.56
1:A:7:LYS:HE2	1:A:35:LYS:HG2	1.86	0.56
1:A:129:THR:OG1	1:A:132:GLU:HG2	2.05	0.56
1:A:289:GLU:HB2	4:A:487:HOH:O	2.04	0.56
1:A:129:THR:HB	1:A:131:GLU:OE1	2.05	0.56
1:A:133:ILE:N	1:A:134:PRO:CD	2.68	0.56
1:A:388:ILE:HA	1:A:391:LEU:HD12	1.87	0.56
1:A:29:GLU:HG2	1:A:35:LYS:HA	1.87	0.56
1:A:260:VAL:HG13	1:A:330:ILE:HA	1.87	0.56
1:A:117:ILE:HG22	1:A:218:PHE:CZ	2.41	0.56
1:A:292:GLU:O	1:A:296:LYS:HG2	2.06	0.55
1:A:443:HIS:HA	1:A:446:ILE:HG13	1.88	0.55
1:A:29:GLU:CG	1:A:35:LYS:HA	2.36	0.55
1:A:392:THR:O	1:A:396:VAL:HG23	2.06	0.55
1:A:332:PRO:HD2	1:A:337:MET:HE2	1.88	0.54
1:A:194:THR:HA	1:A:358:VAL:HG21	1.88	0.54
1:A:384:VAL:O	1:A:387:ASP:HB2	2.07	0.54
1:A:16:LYS:NZ	1:A:112:GLU:OE2	2.41	0.54
1:A:278:LYS:HE2	1:A:282:GLU:OE1	2.07	0.54
1:A:90:LEU:HD11	1:A:286:LEU:HD23	1.89	0.53
1:A:260:VAL:CG1	1:A:330:ILE:HA	2.36	0.53
1:A:291:LEU:HD11	1:A:305:LEU:HB2	1.88	0.53
1:A:169:ALA:O	1:A:182:VAL:HA	2.08	0.53
1:A:382:HIS:O	1:A:385:ASP:HB2	2.09	0.53
1:A:184:VAL:O	1:A:184:VAL:HG12	2.09	0.53
1:A:194:THR:CG2	1:A:358:VAL:HG11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HA	1:A:24:VAL:HG12	1.92	0.52
1:A:418:LEU:HD12	1:A:418:LEU:O	2.09	0.52
1:A:231:TRP:O	1:A:298:LYS:HG3	2.09	0.52
1:A:449:GLU:O	1:A:450:ARG:C	2.52	0.52
1:A:113:ALA:HB2	1:A:325:ALA:HB2	1.91	0.52
1:A:30:LYS:O	1:A:31:ASP:HB2	2.10	0.51
1:A:399:HIS:CD2	1:A:444:VAL:HG21	2.46	0.51
1:A:11:TRP:O	1:A:62:PHE:HB2	2.11	0.51
1:A:115:SER:HB2	4:A:468:HOH:O	2.10	0.51
1:A:130:TRP:HA	1:A:133:ILE:HD13	1.91	0.51
1:A:210:ASP:OD1	1:A:213:ILE:HG12	2.11	0.51
1:A:83:ASP:O	1:A:85:ALA:N	2.43	0.51
1:A:7:LYS:HE2	1:A:35:LYS:HE3	1.93	0.51
1:A:47:LYS:O	1:A:51:VAL:HG22	2.10	0.51
1:A:117:ILE:HB	1:A:226:THR:HG22	1.93	0.51
1:A:261:GLY:HA3	1:A:331:MET:HE3	1.92	0.50
1:A:444:VAL:O	1:A:448:GLN:HG2	2.11	0.50
1:A:258:PRO:HD2	1:A:328:GLY:CA	2.42	0.49
1:A:443:HIS:CD2	1:A:443:HIS:H	2.31	0.49
1:A:200:ILE:HG23	1:A:205:MET:O	2.13	0.49
1:A:194:THR:HG22	1:A:358:VAL:HG11	1.94	0.49
1:A:228:ASN:HD22	1:A:229:GLY:H	1.61	0.48
1:A:421:TRP:C	1:A:423:GLN:H	2.21	0.48
1:A:248:LEU:H	1:A:324:ASN:HD21	1.62	0.48
1:A:21:LEU:HD23	1:A:38:VAL:CG1	2.43	0.48
1:A:109:ILE:HB	1:A:263:LEU:HD23	1.96	0.48
1:A:119:ASN:OD1	1:A:119:ASN:C	2.57	0.48
1:A:21:LEU:HD23	1:A:38:VAL:HG11	1.95	0.48
1:A:261:GLY:CA	1:A:331:MET:HE3	2.43	0.48
1:A:292:GLU:HG3	1:A:308:TYR:OH	2.13	0.48
1:A:403:LEU:O	1:A:407:GLN:HG2	2.13	0.47
1:A:437:LEU:C	1:A:439:ILE:HD12	2.40	0.47
1:A:22:ALA:O	1:A:26:LYS:HD3	2.15	0.47
1:A:134:PRO:HB3	1:A:204:HIS:CE1	2.49	0.47
1:A:15:ASP:OD1	1:A:16:LYS:HD2	2.14	0.47
1:A:80:ILE:HG22	1:A:267:ILE:CD1	2.45	0.47
1:A:90:LEU:HD21	1:A:286:LEU:HD21	1.97	0.47
1:A:339:ALA:O	1:A:340:PHE:C	2.57	0.47
1:A:441:ASN:O	1:A:444:VAL:HB	2.14	0.47
1:A:271:SER:O	1:A:274:LYS:HG3	2.14	0.46
1:A:225:MET:HE3	1:A:225:MET:HB2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HG3	1:A:136:LEU:HD22	1.98	0.46
1:A:443:HIS:HA	1:A:446:ILE:CG1	2.45	0.46
1:A:223:THR:HG22	1:A:225:MET:H	1.80	0.46
1:A:273:ASN:HB3	1:A:276:LEU:HD13	1.96	0.46
1:A:230:PRO:HB3	1:A:299:PRO:HB2	1.97	0.46
1:A:372:MET:CE	1:A:376:SER:HB2	2.42	0.46
1:A:193:LEU:O	1:A:197:VAL:HG23	2.16	0.46
1:A:240:LYS:O	1:A:240:LYS:HG3	2.15	0.46
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.51	0.46
1:A:111:VAL:HB	1:A:302:ALA:HB3	1.98	0.46
1:A:147:ALA:O	1:A:225:MET:HB2	2.16	0.45
1:A:27:LYS:O	1:A:31:ASP:HB3	2.16	0.45
1:A:203:LYS:N	1:A:203:LYS:HE3	2.32	0.45
1:A:118:TYR:HA	1:A:224:ALA:O	2.15	0.45
1:A:117:ILE:HB	1:A:226:THR:HG23	1.99	0.45
1:A:368:ASN:C	1:A:370:ALA:H	2.25	0.45
1:A:137:ASP:HA	1:A:147:ALA:HB2	1.98	0.45
1:A:453:LEU:C	1:A:455:ASN:H	2.24	0.45
1:A:63:TRP:CD1	1:A:64:ALA:H	2.35	0.45
1:A:61:ILE:O	1:A:265:ALA:HA	2.17	0.45
1:A:427:CYS:HB2	4:A:489:HOH:O	2.16	0.45
1:A:12:ILE:HG13	1:A:13:ASN:H	1.82	0.44
1:A:7:LYS:HD3	1:A:35:LYS:O	2.18	0.44
1:A:44:LEU:HD11	1:A:61:ILE:HD11	1.99	0.44
1:A:63:TRP:CD1	1:A:64:ALA:N	2.86	0.44
1:A:193:LEU:HB3	1:A:358:VAL:HG13	1.99	0.44
1:A:271:SER:O	1:A:274:LYS:NZ	2.46	0.44
1:A:102:GLY:O	1:A:103:LYS:HG2	2.17	0.44
1:A:7:LYS:O	1:A:8:LEU:HB2	2.18	0.43
1:A:178:ASP:HB3	1:A:181:ASP:HB3	2.00	0.43
1:A:223:THR:HG22	1:A:224:ALA:N	2.32	0.43
1:A:13:ASN:HD22	1:A:13:ASN:HA	1.65	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.87	0.43
1:A:80:ILE:HD12	1:A:82:PRO:HG3	1.99	0.43
1:A:229:GLY:HA3	1:A:231:TRP:CH2	2.54	0.43
1:A:67:ARG:HG3	1:A:71:TYR:CE2	2.53	0.42
1:A:385:ASP:C	1:A:387:ASP:N	2.73	0.42
1:A:173:GLU:CD	1:A:178:ASP:HB2	2.44	0.42
1:A:80:ILE:HG13	1:A:82:PRO:HD3	2.00	0.42
1:A:355:ARG:HA	1:A:355:ARG:HD3	1.70	0.42
1:A:32:THR:CG2	1:A:34:ILE:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TRP:N	1:A:160:PRO:CD	2.83	0.42
1:A:62:PHE:CE2	1:A:265:ALA:HB2	2.55	0.42
1:A:255:PRO:HB2	1:A:327:LYS:HG2	2.00	0.42
1:A:102:GLY:C	1:A:103:LYS:HG2	2.45	0.42
1:A:330:ILE:O	1:A:330:ILE:HG23	2.19	0.42
1:A:133:ILE:N	1:A:133:ILE:HD12	2.34	0.42
1:A:314:LYS:HA	1:A:314:LYS:HD3	1.67	0.42
1:A:336:GLN:HE21	1:A:336:GLN:HB2	1.65	0.42
1:A:8:LEU:HD13	1:A:276:LEU:HB3	2.02	0.42
1:A:385:ASP:O	1:A:386:LYS:C	2.63	0.41
1:A:407:GLN:HG2	1:A:407:GLN:H	1.53	0.41
1:A:48:PHE:N	1:A:49:PRO:HD2	2.34	0.41
1:A:230:PRO:CB	1:A:299:PRO:HB2	2.50	0.41
1:A:281:LEU:O	1:A:286:LEU:HB2	2.21	0.41
1:A:223:THR:CG2	1:A:224:ALA:N	2.83	0.41
1:A:303:VAL:O	1:A:309:GLU:HG2	2.21	0.41
1:A:21:LEU:HA	1:A:24:VAL:CG1	2.51	0.41
1:A:230:PRO:O	1:A:232:ALA:N	2.54	0.41
1:A:364:ALA:O	1:A:365:ALA:C	2.64	0.41
1:A:23:GLU:C	1:A:25:GLY:N	2.77	0.40
1:A:46:GLU:O	1:A:49:PRO:HG2	2.20	0.40
1:A:109:ILE:HG12	1:A:264:SER:HA	2.02	0.40
1:A:147:ALA:O	1:A:225:MET:N	2.54	0.40
1:A:114:LEU:HD22	1:A:227:ILE:HG22	2.02	0.40
1:A:125:ASN:ND2	1:A:125:ASN:C	2.79	0.40
1:A:232:ALA:O	1:A:233:TRP:C	2.65	0.40
1:A:375:ALA:O	1:A:378:LYS:HB2	2.22	0.40
1:A:77:LEU:C	1:A:269:ALA:HB2	2.46	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 X-ray entries followed by that with respect to entries of similar resolution.

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	448/450 (100%)	390 (87%)	46 (10%)	12 (3%)	4 6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	84	LYS
1	A	169	ALA
1	A	8	LEU
1	A	29	GLU
1	A	231	TRP
1	A	233	TRP
1	A	32	THR
1	A	286	LEU
1	A	303	VAL
1	A	381	LEU
1	A	450	ARG

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 X-ray entries followed by that with respect to entries of similar resolution.

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	361/361 (100%)	288 (80%)	73 (20%)	1 2

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	10	ILE
1	A	12	ILE
1	A	13	ASN
1	A	16	LYS
1	A	24	VAL
1	A	26	LYS
1	A	29	GLU
1	A	32	THR

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Mol	Chain	Res	Type
1	A	36	VAL
1	A	37	THR
1	A	47	LYS
1	A	51	VAL
1	A	67	ARG
1	A	77	LEU
1	A	81	THR
1	A	83	ASP
1	A	115	SER
1	A	119	ASN
1	A	120	LYS
1	A	125	ASN
1	A	128	LYS
1	A	136	LEU
1	A	138	LYS
1	A	139	GLU
1	A	141	LYS
1	A	143	LYS
1	A	145	LYS
1	A	146	SER
1	A	149	MET
1	A	153	GLN
1	A	158	THR
1	A	171	LYS
1	A	196	LEU
1	A	199	LEU
1	A	203	LYS
1	A	208	ASP
1	A	209	THR
1	A	220	LYS
1	A	222	GLU
1	A	225	MET
1	A	228	ASN
1	A	242	ASN
1	A	252	LYS
1	A	257	LYS
1	A	259	PHE
1	A	263	LEU
1	A	273	ASN
1	A	275	GLU
1	A	278	LYS
1	A	292	GLU

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	298	LYS
1	A	306	LYS
1	A	307	SER
1	A	309	GLU
1	A	310	GLU
1	A	317	ARG
1	A	327	LYS
1	A	329	GLU
1	A	336	GLN
1	A	393	GLN
1	A	400	LYS
1	A	404	LYS
1	A	407	GLN
1	A	413	ARG
1	A	422	GLU
1	A	423	GLN
1	A	434	CYS
1	A	438	ASN
1	A	439	ILE
1	A	448	GLN
1	A	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	19	ASN
1	A	73	GLN
1	A	202	ASN
1	A	219	ASN
1	A	228	ASN
1	A	235	ASN
1	A	254	GLN
1	A	324	ASN
1	A	336	GLN
1	A	368	ASN
1	A	399	HIS
1	A	441	ASN
1	A	443	HIS

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
2	GLC	B	1	2	12,12,12	0.94	1 (8%)	17,17,17	2.07	6 (35%)
2	GLC	B	2	2	11,11,12	1.42	2 (18%)	15,15,17	1.30	1 (6%)

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
2	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	C4-C5	2.34	1.58	1.53
2	B	2	GLC	O5-C1	-2.25	1.39	1.43
2	B	2	GLC	O5-C5	2.06	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C1-O5-C5	5.41	124.11	113.65
2	B	2	GLC	C1-O5-C5	4.06	117.63	112.19
2	B	1	GLC	O1-C1-O5	-3.29	100.65	110.41
2	B	1	GLC	O5-C1-C2	2.78	115.18	110.30
2	B	1	GLC	O6-C6-C5	-2.57	102.57	111.33
2	B	1	GLC	O5-C5-C6	2.33	112.22	106.44
2	B	1	GLC	O3-C3-C2	-2.06	105.52	110.38

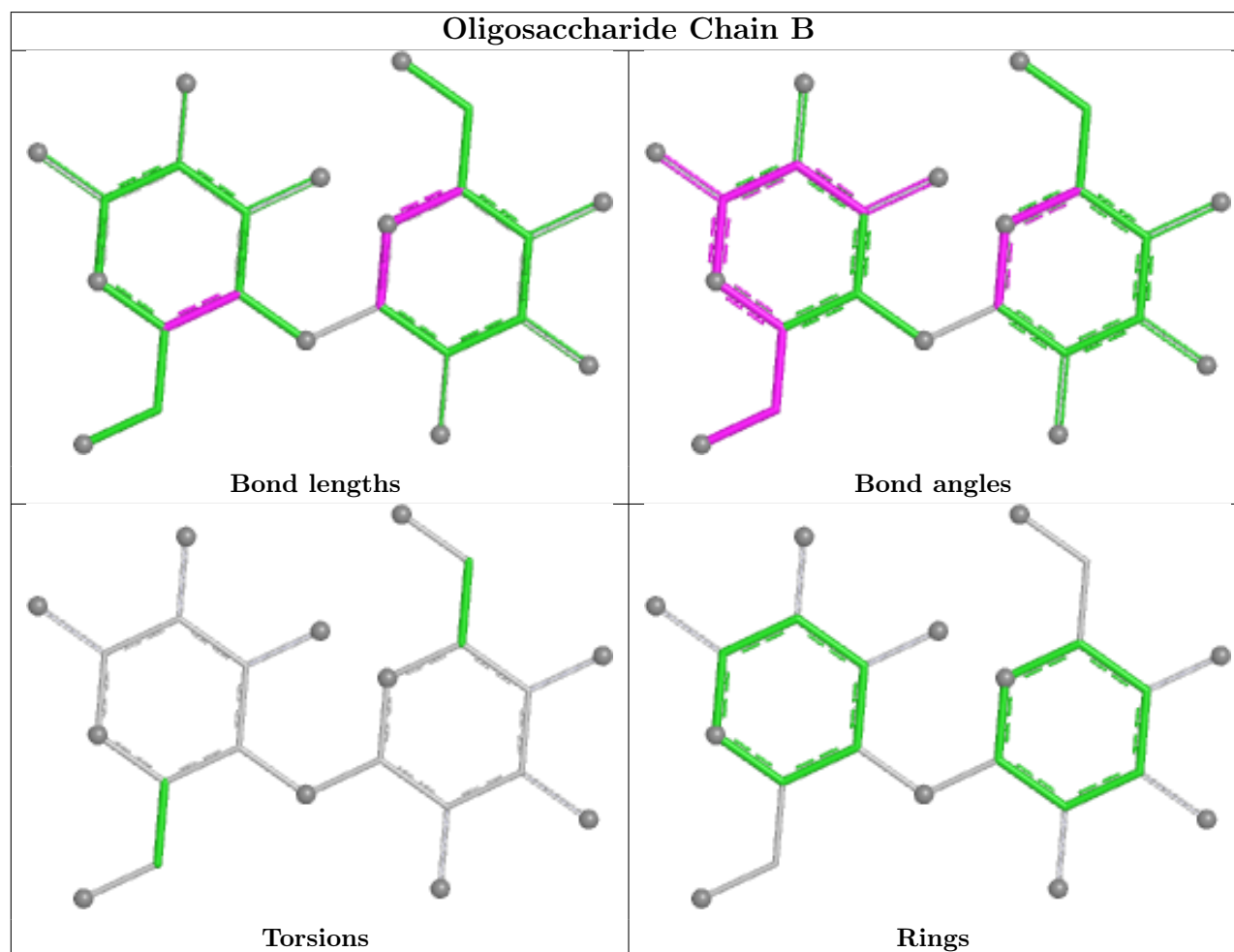
There are no chirality outliers.

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 oligosaccharide.



5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.