



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:31 AM UTC

PDB ID : 1PNV / pdb_00001pnv
Title : Crystal Structure of TDP-epi-Vancosaminyltransferase GtfA in complexes with TDP and Vancomycin
Authors : Mulichak, A.M.; Losey, H.C.; Lu, W.; Wawrzak, Z.; Walsh, C.T.; Garavito, R.M.
Deposited on : 2003-06-13
Resolution : 2.80 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

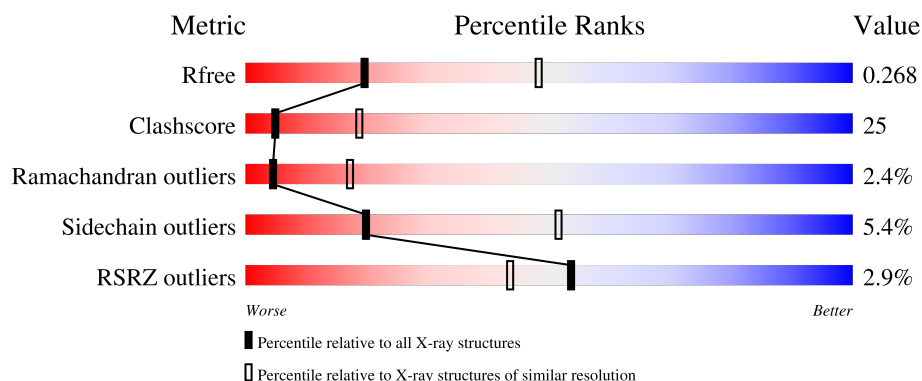
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

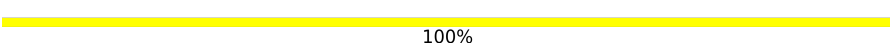
The reported resolution of this entry is 2.80 Å.

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	
2	C	7	
3	D	2	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5783 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 GLYCOSYLTRANSFERASE GTFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2787	1757	490	528	12			
1	B	384	Total	C	N	O	S	0	0	0
			2784	1749	493	530	12			

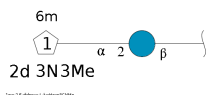
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	LEU	-	expression tag	UNP P96558
A	398	GLU	-	expression tag	UNP P96558
A	399	HIS	-	expression tag	UNP P96558
A	400	HIS	-	expression tag	UNP P96558
A	401	HIS	-	expression tag	UNP P96558
A	402	HIS	-	expression tag	UNP P96558
A	403	HIS	-	expression tag	UNP P96558
A	404	HIS	-	expression tag	UNP P96558
B	397	LEU	-	expression tag	UNP P96558
B	398	GLU	-	expression tag	UNP P96558
B	399	HIS	-	expression tag	UNP P96558
B	400	HIS	-	expression tag	UNP P96558
B	401	HIS	-	expression tag	UNP P96558
B	402	HIS	-	expression tag	UNP P96558
B	403	HIS	-	expression tag	UNP P96558
B	404	HIS	-	expression tag	UNP P96558

- Molecule 2 is a protein called VANCOMYCIN.

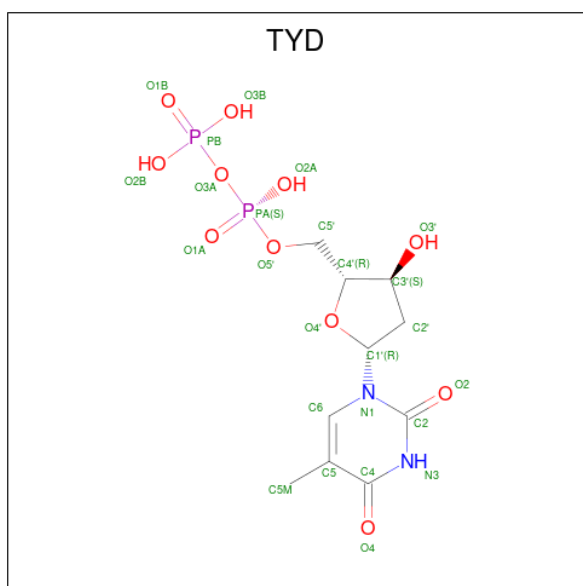
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			

- Molecule 3 is an oligosaccharide called vancosamine-(1-2)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			21	13	1	7			

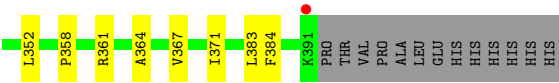
- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (CCD ID: TYD) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}_{11}\text{P}_2$).



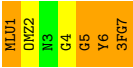
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is water.

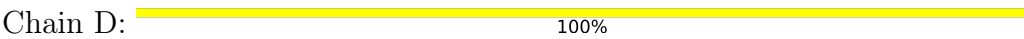
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	43	Total O 43 43	0	0
5	C	7	Total O 7 7	0	0



● Molecule 2: VANCOMYCIN



● Molecule 3: vancosamine-(1-2)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.17Å 153.17Å 100.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.80) 94.6 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.269 0.226 , 0.268	Depositor DCC
R_{free} test set	1686 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5783	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMY, TYD, 3FG, GHP, MLU, OMZ, BGC, RER

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	0.46	0/2843	1.01	11/3894 (0.3%)
1	B	0.51	0/2839	1.00	12/3891 (0.3%)
2	C	1.05	0/7	1.65	0/8
All	All	0.49	0/5689	1.00	23/7793 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLY	N-CA-C	-9.45	101.84	111.85
1	B	339	ASP	N-CA-C	7.60	118.30	108.34
1	A	182	ASP	CA-C-N	7.33	126.86	119.24
1	A	182	ASP	C-N-CA	7.33	126.86	119.24
1	A	39	TYR	N-CA-C	7.12	120.83	112.72
1	A	223	PRO	N-CA-C	6.71	121.13	111.13
1	B	157	ARG	N-CA-C	-6.62	104.15	111.36
1	A	222	THR	CA-C-N	6.45	126.90	120.52
1	A	222	THR	C-N-CA	6.45	126.90	120.52
1	A	132	GLU	N-CA-C	-6.42	104.06	112.41
1	B	244	ILE	N-CA-C	-5.80	104.85	110.42
1	B	46	VAL	N-CA-C	-5.78	108.22	113.71
1	A	220	GLY	N-CA-C	5.52	118.22	110.38
1	A	136	ALA	N-CA-C	-5.51	104.74	112.12
1	B	313	ARG	N-CA-C	5.47	118.21	110.50
1	A	375	GLY	N-CA-C	5.42	119.20	112.64
1	B	220	GLY	N-CA-C	5.32	118.02	110.74
1	B	89	ALA	N-CA-C	5.30	117.06	111.28
1	B	291	ILE	N-CA-C	-5.16	100.32	107.80
1	B	265	LEU	CA-C-N	5.13	126.25	119.84
1	B	265	LEU	C-N-CA	5.13	126.25	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LEU	N-CA-C	-5.09	103.68	110.55
1	B	255	VAL	N-CA-C	-5.04	98.70	106.72

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	2787	0	2763	146	0
1	B	2784	0	2742	138	0
2	C	80	0	45	8	0
3	D	21	0	21	1	0
4	A	25	0	13	4	0
5	A	36	0	0	4	0
5	B	43	0	0	1	0
5	C	7	0	0	0	0
All	All	5783	0	5584	285	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 25.

All (285) 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:87:PRO:HD3	1:A:111:MET:HE1	1.33	1.04
1:B:345:ILE:HD12	1:B:345:ILE:H	1.20	1.03
1:B:17:LEU:HD11	1:B:99:THR:HG22	1.42	1.01
1:A:185:LEU:HD13	1:A:303:MET:HE1	1.46	0.96
1:A:6:THR:HG22	1:A:34:CYS:HB2	1.52	0.90
1:A:389:LEU:HD21	1:B:212:GLU:HG2	1.54	0.89
1:A:240:ALA:O	1:A:244:ILE:HG12	1.73	0.88
1:B:303:MET:HE2	1:B:371:ILE:HD11	1.54	0.88
1:B:202:ILE:HD12	1:B:304:ARG:NH1	1.89	0.88
1:A:131:SER:OG	1:A:192:ASP:HB3	1.74	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HG	1:A:274:VAL:HG22	1.58	0.85
1:A:179:LEU:HD23	1:A:197:GLN:HE21	1.43	0.84
1:A:209:LEU:HB3	1:A:213:LEU:HD23	1.61	0.80
1:B:260:TRP:HZ2	1:B:277:GLU:HG3	1.49	0.77
1:A:173:TYR:O	1:A:177:PRO:HG3	1.84	0.77
1:B:86:VAL:HB	1:B:111:MET:HE3	1.66	0.77
1:A:329:VAL:HG13	1:A:334:VAL:HG23	1.66	0.76
1:A:244:ILE:HD12	1:A:254:ILE:CD1	2.16	0.76
1:A:87:PRO:CD	1:A:111:MET:HE1	2.13	0.75
1:A:252:ARG:CZ	1:A:356:LEU:HD13	2.18	0.74
1:B:173:TYR:O	1:B:174:THR:HB	1.88	0.73
1:B:101:LEU:HG	1:B:103:PRO:HD2	1.70	0.73
1:B:13:ASP:HA	1:B:124:LEU:HD11	1.71	0.73
1:B:242:MET:SD	1:B:345:ILE:HG13	2.30	0.72
1:B:189:ARG:HB3	1:B:190:PRO:HD2	1.71	0.70
1:A:212:GLU:OE1	1:A:212:GLU:N	2.24	0.70
1:A:179:LEU:HD23	1:A:197:GLN:NE2	2.06	0.69
1:A:6:THR:CG2	1:A:34:CYS:HB2	2.22	0.69
1:A:17:LEU:HD11	1:A:99:THR:HG22	1.74	0.69
1:A:75:VAL:CG1	1:A:149:PHE:HB3	2.22	0.69
1:A:32:ARG:HD3	5:A:2002:HOH:O	1.92	0.69
1:B:176:GLN:NE2	1:B:194:GLY:O	2.26	0.68
1:B:72:ALA:HB2	2:C:1:MLU:HD12	1.73	0.68
1:B:2:ARG:HA	1:B:30:ASP:O	1.94	0.68
1:A:134:SER:OG	1:A:137:GLU:HG2	1.93	0.68
1:B:75:VAL:HG21	1:B:148:LEU:HD11	1.76	0.67
1:B:345:ILE:HD12	1:B:345:ILE:N	2.02	0.67
1:B:17:LEU:HD11	1:B:99:THR:CG2	2.24	0.67
1:A:332:LEU:O	1:A:363:ARG:HD3	1.93	0.66
1:B:345:ILE:H	1:B:345:ILE:CD1	1.98	0.66
1:A:74:VAL:HG23	1:A:77:GLU:HB3	1.76	0.65
1:A:134:SER:C	1:A:136:ALA:H	2.04	0.65
1:A:36:PRO:HG2	1:A:39:TYR:HE1	1.62	0.64
1:A:98:THR:HG22	1:A:99:THR:N	2.12	0.64
1:A:2:ARG:HH11	1:A:2:ARG:HG2	1.61	0.64
1:A:58:ARG:HG3	1:A:260:TRP:CD2	2.34	0.63
1:A:86:VAL:N	1:A:87:PRO:HD2	2.14	0.63
1:B:72:ALA:O	1:B:75:VAL:HG23	1.99	0.63
1:B:334:VAL:HG22	1:B:364:ALA:HA	1.80	0.63
1:A:247:VAL:HG22	1:A:352:LEU:HD11	1.80	0.62
1:B:90:ILE:HD11	1:B:117:ILE:HD11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG23	1:A:41:GLU:N	2.14	0.61
1:A:149:PHE:CE1	1:A:168:LEU:HD23	2.36	0.61
1:B:146:ASP:OD2	1:B:168:LEU:HG	2.00	0.61
1:B:1:MET:HE3	1:B:3:VAL:HG22	1.82	0.61
1:A:176:GLN:HE22	1:A:195:THR:HG22	1.66	0.60
1:A:252:ARG:NH1	1:A:356:LEU:HD13	2.17	0.60
1:B:202:ILE:HD11	1:B:300:LEU:HD23	1.83	0.60
1:B:247:VAL:HG11	1:B:254:ILE:HG12	1.84	0.60
1:A:297:GLY:HA3	4:A:405:TYD:O1A	2.03	0.59
1:B:75:VAL:HG11	1:B:149:PHE:HB3	1.84	0.59
1:A:74:VAL:HG22	1:A:78:VAL:HG23	1.83	0.59
1:B:202:ILE:HD12	1:B:304:ARG:CZ	2.33	0.59
1:B:1:MET:HE3	1:B:3:VAL:CG2	2.32	0.58
1:B:157:ARG:HH12	1:B:162:LEU:HB3	1.67	0.58
1:A:183:PRO:HA	1:A:197:GLN:OE1	2.04	0.58
1:B:240:ALA:O	1:B:244:ILE:HG12	2.02	0.58
1:A:327:ASP:O	1:A:331:GLU:HG3	2.01	0.58
1:B:75:VAL:CG1	1:B:149:PHE:HB3	2.33	0.58
1:A:36:PRO:HG2	1:A:39:TYR:CE1	2.37	0.58
1:B:6:THR:HG22	1:B:34:CYS:HB2	1.86	0.57
1:B:269:GLY:C	1:B:271:ASP:H	2.13	0.57
1:B:84:ASP:O	1:B:87:PRO:HD2	2.04	0.57
1:B:158:ALA:C	1:B:160:ILE:H	2.13	0.57
1:A:244:ILE:HD12	1:A:254:ILE:HD11	1.86	0.57
1:A:244:ILE:HG23	1:A:254:ILE:HD13	1.86	0.56
1:A:101:LEU:HG	1:A:103:PRO:HG2	1.85	0.56
1:B:22:ALA:O	1:B:26:GLU:HG3	2.06	0.56
1:A:175:ASP:O	1:A:176:GLN:HG2	2.05	0.56
1:B:345:ILE:O	1:B:349:SER:HB2	2.06	0.56
1:A:45:GLU:OE1	1:A:207:ARG:HD3	2.06	0.56
1:B:51:VAL:HG11	1:B:89:ALA:HB2	1.88	0.56
1:A:54:GLY:HA2	1:A:81:GLU:OE1	2.06	0.56
1:A:265:LEU:CG	1:A:274:VAL:HG22	2.33	0.55
1:B:303:MET:HB3	1:B:371:ILE:CD1	2.37	0.55
1:A:243:ALA:O	1:A:247:VAL:HG23	2.07	0.55
1:A:343:PRO:HG2	1:A:348:LEU:HD11	1.87	0.55
1:B:260:TRP:CZ2	1:B:277:GLU:HG3	2.37	0.55
1:B:231:SER:OG	1:B:233:ARG:HB2	2.06	0.55
1:B:41:GLU:O	1:B:44:ALA:HB3	2.07	0.55
1:B:101:LEU:HD13	2:C:5:GHP:H6	1.88	0.55
1:B:212:GLU:O	1:B:215:ALA:HB3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HG12	1:B:90:ILE:O	2.07	0.54
1:B:10:SER:HB3	2:C:6:OMY:O	2.08	0.54
1:A:154:ASN:HD22	1:A:154:ASN:H	1.55	0.54
1:B:303:MET:HE3	1:B:367:VAL:HG11	1.89	0.54
1:A:187:PRO:HG2	5:A:2014:HOH:O	2.08	0.54
1:A:300:LEU:HD12	5:A:2013:HOH:O	2.07	0.54
1:B:244:ILE:HD11	1:B:256:LEU:HD13	1.88	0.54
2:C:6:OMY:CL	3:D:2:RER:H5A2	2.44	0.54
1:B:216:PHE:O	1:B:253:ARG:NH2	2.38	0.53
1:B:269:GLY:O	1:B:271:ASP:N	2.41	0.53
1:A:15:GLU:N	1:A:16:PRO:HD2	2.23	0.53
1:A:389:LEU:HD21	1:B:212:GLU:CG	2.33	0.53
1:A:313:ARG:HG3	1:A:314:ARG:H	1.73	0.53
1:A:149:PHE:CD1	1:A:168:LEU:HD23	2.44	0.53
1:B:60:GLY:C	1:B:62:ARG:H	2.17	0.53
1:B:310:ILE:HD11	1:B:352:LEU:HA	1.90	0.53
1:A:2:ARG:HD3	1:A:32:ARG:HH12	1.74	0.52
1:B:157:ARG:HH11	1:B:157:ARG:HB3	1.74	0.52
1:A:179:LEU:CD2	1:A:197:GLN:NE2	2.71	0.52
1:A:188:LEU:HD22	1:A:192:ASP:OD2	2.10	0.52
1:A:87:PRO:HA	1:A:90:ILE:HG22	1.91	0.52
1:B:174:THR:HG22	1:B:176:GLN:N	2.25	0.52
1:B:275:VAL:HG22	1:B:278:VAL:HB	1.92	0.51
1:B:52:PRO:O	1:B:53:VAL:HG23	2.10	0.51
1:B:296:ALA:HB2	1:B:325:HIS:NE2	2.25	0.51
1:A:200:ALA:O	1:A:375:GLY:HA3	2.11	0.51
1:B:158:ALA:O	1:B:160:ILE:N	2.43	0.51
1:B:243:ALA:O	1:B:247:VAL:HG23	2.10	0.51
1:B:258:ARG:NH1	1:B:262:ASP:HB3	2.26	0.51
1:A:98:THR:CG2	1:A:99:THR:N	2.74	0.51
1:A:74:VAL:O	1:A:77:GLU:N	2.41	0.51
1:A:157:ARG:HH21	1:A:162:LEU:HD22	1.75	0.51
1:A:235:ALA:HB1	1:A:341:PRO:HB2	1.93	0.51
1:A:235:ALA:CB	1:A:341:PRO:HB2	2.41	0.51
1:B:40:VAL:HG23	1:B:41:GLU:N	2.25	0.51
1:A:12:GLY:HA2	4:A:405:TYD:C5'	2.41	0.51
1:A:142:ASN:OD1	1:A:169:TYR:HB3	2.11	0.50
1:A:202:ILE:HD11	1:A:300:LEU:HD21	1.93	0.50
1:A:334:VAL:HG12	1:A:364:ALA:HA	1.92	0.50
1:B:153:VAL:HG12	1:B:157:ARG:HD2	1.93	0.50
1:A:310:ILE:HD11	1:A:352:LEU:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:OD1	1:A:164:PRO:HB3	2.12	0.50
1:B:174:THR:HG22	1:B:176:GLN:H	1.77	0.50
1:A:2:ARG:HG2	1:A:2:ARG:NH1	2.27	0.49
1:B:150:GLY:HA2	1:B:168:LEU:HD11	1.93	0.49
1:A:265:LEU:HG	1:A:274:VAL:CG2	2.39	0.49
1:A:40:VAL:CG2	1:A:41:GLU:N	2.76	0.49
1:B:339:ASP:OD2	1:B:339:ASP:C	2.54	0.49
1:A:106:VAL:HG13	1:A:171:TYR:HD2	1.77	0.49
1:B:94:ASP:O	1:B:118:PRO:HD2	2.11	0.49
1:A:35:LEU:HB2	1:A:50:MET:HE2	1.95	0.49
1:B:102:LEU:HB3	1:B:103:PRO:HD3	1.93	0.49
1:B:278:VAL:HG22	1:B:279:ASN:N	2.28	0.49
1:A:56:ALA:HB3	1:A:62:ARG:HG3	1.95	0.49
1:A:150:GLY:O	1:A:154:ASN:ND2	2.40	0.49
1:B:13:ASP:HA	1:B:124:LEU:CD1	2.43	0.49
1:A:154:ASN:H	1:A:154:ASN:ND2	2.11	0.49
1:B:87:PRO:HD3	1:B:111:MET:HE3	1.94	0.49
1:A:363:ARG:O	1:A:363:ARG:HG3	2.13	0.49
1:A:134:SER:C	1:A:136:ALA:N	2.71	0.48
1:B:86:VAL:HB	1:B:111:MET:CE	2.39	0.48
2:C:5:GHP:C2	2:C:7:3FG:HN1	2.26	0.48
1:B:329:VAL:CG1	1:B:335:GLY:HA3	2.43	0.48
1:B:83:PHE:O	1:B:111:MET:HE1	2.13	0.48
1:A:12:GLY:HA2	4:A:405:TYD:H5'2	1.94	0.48
1:A:37:PRO:HG2	1:A:56:ALA:HA	1.94	0.48
1:A:202:ILE:HD11	1:A:300:LEU:CD2	2.43	0.48
1:A:238:ASP:O	1:A:242:MET:HG2	2.14	0.48
1:B:32:ARG:HA	1:B:49:PRO:HG2	1.95	0.47
1:B:127:ASP:OD1	1:B:127:ASP:N	2.46	0.47
1:B:4:LEU:HD22	1:B:90:ILE:HB	1.95	0.47
1:B:98:THR:HG22	1:B:99:THR:N	2.29	0.47
1:A:176:GLN:NE2	1:A:195:THR:HG22	2.29	0.47
1:A:14:THR:C	1:A:16:PRO:HD2	2.40	0.47
1:B:40:VAL:HA	1:B:50:MET:HE3	1.95	0.47
1:B:174:THR:CG2	1:B:176:GLN:H	2.28	0.47
1:A:189:ARG:C	1:A:191:THR:H	2.23	0.47
1:B:334:VAL:HG21	1:B:367:VAL:HG21	1.97	0.47
1:A:149:PHE:O	1:A:150:GLY:C	2.58	0.47
1:A:160:ILE:HD11	1:A:162:LEU:HD12	1.97	0.47
1:A:74:VAL:CG2	1:A:77:GLU:HB3	2.44	0.46
1:B:258:ARG:NH1	1:B:263:LEU:O	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HA	1:B:50:MET:CE	2.45	0.46
1:A:146:ASP:O	1:A:150:GLY:HA3	2.16	0.46
1:A:309:GLN:O	1:A:335:GLY:HA3	2.16	0.46
1:B:209:LEU:HB2	1:B:214:GLU:OE2	2.16	0.46
1:B:220:GLY:C	1:B:253:ARG:NH1	2.73	0.46
1:A:57:VAL:HG23	1:A:260:TRP:CH2	2.50	0.46
1:B:313:ARG:NH1	1:B:327:ASP:OD1	2.47	0.46
1:A:2:ARG:HB2	1:A:93:CYS:HA	1.98	0.46
1:B:126:PRO:HA	1:B:129:LEU:HG	1.97	0.46
1:A:74:VAL:O	1:A:75:VAL:C	2.58	0.46
1:A:59:ALA:HA	1:A:62:ARG:NH2	2.31	0.46
1:A:325:HIS:O	1:A:329:VAL:HG23	2.15	0.46
1:A:351:ALA:C	1:A:353:ASP:N	2.73	0.46
1:A:2:ARG:HD2	1:A:92:GLY:O	2.15	0.46
1:A:154:ASN:HA	1:A:157:ARG:HB2	1.97	0.46
1:A:176:GLN:HE21	1:A:176:GLN:HA	1.81	0.46
1:A:109:ARG:NH1	1:A:174:THR:HG22	2.31	0.46
1:B:124:LEU:O	1:B:181:ALA:HB2	2.16	0.45
1:B:325:HIS:O	1:B:326:ALA:C	2.60	0.45
1:B:32:ARG:HD3	1:B:49:PRO:CG	2.46	0.45
1:B:101:LEU:HD13	2:C:5:GHP:C6	2.46	0.45
1:A:75:VAL:HG12	1:A:149:PHE:HB3	1.98	0.45
1:B:268:ASP:O	1:B:269:GLY:C	2.59	0.45
1:A:72:ALA:O	1:A:75:VAL:HG23	2.16	0.45
1:B:86:VAL:HG11	1:B:111:MET:HG3	1.99	0.45
1:B:109:ARG:HD3	1:B:171:TYR:CZ	2.51	0.45
1:A:324:TYR:O	1:A:328:ARG:HG2	2.17	0.45
2:C:5:GHP:C2	2:C:7:3FG:N	2.80	0.45
1:A:184:VAL:HG21	1:A:370:THR:OG1	2.17	0.45
1:B:158:ALA:C	1:B:160:ILE:N	2.75	0.45
1:A:72:ALA:HA	1:A:75:VAL:HG23	1.98	0.45
1:A:311:VAL:HG11	1:A:326:ALA:HA	1.99	0.45
1:B:25:ARG:O	1:B:28:GLY:N	2.47	0.45
1:A:101:LEU:HG	1:A:103:PRO:CG	2.47	0.45
1:B:269:GLY:C	1:B:271:ASP:N	2.73	0.45
1:B:51:VAL:HG13	1:B:51:VAL:O	2.17	0.44
1:B:73:GLU:H	1:B:73:GLU:CD	2.25	0.44
1:A:134:SER:O	1:A:136:ALA:N	2.43	0.44
1:B:344:THR:OG1	1:B:347:SER:HB2	2.18	0.44
1:B:358:PRO:HA	1:B:361:ARG:HD3	2.00	0.44
1:B:86:VAL:N	1:B:87:PRO:CD	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HG11	1:B:283:LEU:HD21	1.99	0.44
1:A:46:VAL:HG12	1:A:46:VAL:O	2.17	0.44
1:A:297:GLY:CA	4:A:405:TYD:O1A	2.66	0.44
1:B:185:LEU:HD13	1:B:303:MET:SD	2.57	0.44
1:B:303:MET:HB3	1:B:371:ILE:HD11	1.99	0.44
1:A:244:ILE:CD1	1:A:254:ILE:CD1	2.94	0.44
1:B:52:PRO:O	1:B:53:VAL:CG2	2.66	0.44
1:A:157:ARG:NH2	1:A:162:LEU:HD22	2.33	0.44
1:B:75:VAL:O	1:B:78:VAL:HB	2.18	0.44
1:B:260:TRP:HZ2	1:B:277:GLU:CG	2.25	0.44
1:A:6:THR:O	1:A:98:THR:HA	2.17	0.44
1:A:106:VAL:HG13	1:A:171:TYR:CD2	2.53	0.44
1:B:260:TRP:CZ2	1:B:277:GLU:CG	3.01	0.43
1:A:176:GLN:HE21	1:A:176:GLN:CA	2.29	0.43
1:A:139:ASP:OD1	1:A:139:ASP:N	2.51	0.43
1:B:98:THR:CG2	1:B:99:THR:N	2.81	0.43
1:B:40:VAL:CG1	1:B:50:MET:HE1	2.49	0.43
1:A:86:VAL:N	1:A:87:PRO:CD	2.80	0.43
1:A:241:LYS:HE3	5:A:2020:HOH:O	2.19	0.43
1:A:309:GLN:HG3	1:A:329:VAL:HG11	2.00	0.43
1:A:155:SER:O	1:A:158:ALA:HB3	2.18	0.42
1:B:93:CYS:O	1:B:117:ILE:HG21	2.19	0.42
1:B:248:ARG:HG2	1:B:248:ARG:HH11	1.83	0.42
1:A:157:ARG:O	1:A:162:LEU:HB2	2.19	0.42
1:B:288:ALA:O	1:B:308:PRO:HD2	2.18	0.42
1:B:248:ARG:NH1	1:B:271:ASP:OD2	2.52	0.42
1:A:38:ASP:CG	1:A:57:VAL:HG22	2.43	0.42
1:A:165:VAL:HG23	1:A:168:LEU:HD11	2.01	0.42
1:B:15:GLU:N	1:B:16:PRO:CD	2.83	0.42
1:A:31:ALA:O	1:A:32:ARG:HG2	2.19	0.42
1:B:1:MET:HE2	1:B:384:PHE:CE2	2.54	0.42
1:B:3:VAL:HG13	1:B:95:ALA:HB3	2.00	0.42
1:B:248:ARG:HH12	1:B:271:ASP:CG	2.27	0.42
1:B:160:ILE:HG12	1:B:160:ILE:O	2.20	0.42
1:B:313:ARG:HE	1:B:339:ASP:HB3	1.84	0.42
1:A:333:GLY:O	1:A:363:ARG:HG2	2.19	0.42
1:B:71:ALA:HB3	1:B:74:VAL:HG22	2.02	0.42
1:B:5:ILE:HD12	1:B:21:ALA:HB2	2.02	0.42
1:B:52:PRO:C	1:B:53:VAL:HG23	2.45	0.41
1:A:331:GLU:C	1:A:333:GLY:N	2.78	0.41
1:B:33:MET:HE2	1:B:48:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:VAL:CG1	1:B:111:MET:HG3	2.51	0.41
1:A:98:THR:CG2	1:A:99:THR:H	2.34	0.41
1:B:37:PRO:HG2	1:B:56:ALA:HB2	2.01	0.41
1:B:185:LEU:HD21	1:B:325:HIS:HD2	1.85	0.41
1:A:367:VAL:O	1:A:367:VAL:HG12	2.21	0.41
1:B:130:PRO:HD2	5:B:2013:HOH:O	2.20	0.41
1:B:258:ARG:HG3	1:B:274:VAL:HG13	2.02	0.41
1:A:102:LEU:N	1:A:103:PRO:HD2	2.35	0.41
1:B:83:PHE:HA	1:B:111:MET:HE2	2.02	0.41
1:B:280:LEU:HA	1:B:280:LEU:HD12	1.82	0.41
1:A:21:ALA:O	1:A:25:ARG:HG3	2.21	0.41
1:A:72:ALA:HA	1:A:75:VAL:CG2	2.51	0.41
1:A:150:GLY:HA2	1:A:168:LEU:CD2	2.51	0.41
1:A:354:THR:O	1:A:357:ALA:HB3	2.21	0.41
1:B:157:ARG:NH1	1:B:162:LEU:CB	2.84	0.41
1:A:62:ARG:NH1	1:A:68:PRO:N	2.69	0.41
1:A:213:LEU:O	1:A:217:LEU:HG	2.21	0.41
1:B:157:ARG:HH12	1:B:162:LEU:CB	2.33	0.41
1:A:85:LYS:C	1:A:87:PRO:HD2	2.46	0.40
1:A:267:ASP:C	1:A:269:GLY:H	2.29	0.40
1:A:387:VAL:CG1	1:B:264:VAL:HG22	2.51	0.40
1:B:1:MET:HE1	1:B:383:LEU:HB3	2.03	0.40
1:A:182:ASP:HA	1:A:183:PRO:HD3	1.80	0.40
1:A:284:PHE:CE2	1:A:302:ALA:HB2	2.57	0.40
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.96	0.40
1:A:255:VAL:HG11	1:A:283:LEU:HD21	2.02	0.40
1:B:5:ILE:HB	1:B:33:MET:HG2	2.03	0.40
1:A:157:ARG:HH21	1:A:162:LEU:HB3	1.87	0.40
2:C:1:MLU:HD23	2:C:1:MLU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	378/404 (94%)	343 (91%)	27 (7%)	8 (2%)	5	20
1	B	380/404 (94%)	353 (93%)	17 (4%)	10 (3%)	4	15
2	C	1/7 (14%)	1 (100%)	0	0	100	100
All	All	759/815 (93%)	697 (92%)	44 (6%)	18 (2%)	4	17

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	B	64	PRO
1	B	159	SER
1	B	270	ALA
1	A	150	GLY
1	A	195	THR
1	B	38	ASP
1	B	91	GLU
1	B	219	ALA
1	B	324	TYR
1	A	135	GLN
1	B	61	ALA
1	B	101	LEU
1	A	37	PRO
1	A	190	PRO
1	A	101	LEU
1	B	160	ILE
1	A	341	PRO

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	280/311 (90%)	265 (95%)	15 (5%)	20	51
1	B	278/311 (89%)	263 (95%)	15 (5%)	20	51
2	C	1/1 (100%)	1 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	559/623 (90%)	529 (95%)	30 (5%)	20	51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	73	GLU
1	A	122	THR
1	A	168	LEU
1	A	176	GLN
1	A	186	SER
1	A	192	ASP
1	A	197	GLN
1	A	222	THR
1	A	254	ILE
1	A	274	VAL
1	A	334	VAL
1	A	352	LEU
1	A	363	ARG
1	A	365	THR
1	B	3	VAL
1	B	13	ASP
1	B	64	PRO
1	B	77	GLU
1	B	83	PHE
1	B	94	ASP
1	B	127	ASP
1	B	157	ARG
1	B	174	THR
1	B	280	LEU
1	B	331	GLU
1	B	334	VAL
1	B	338	VAL
1	B	345	ILE
1	B	348	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	GLN
1	B	197	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	MLU	C	1	2	7,8,9	1.51	2 (28%)	7,9,11	0.88	0
2	GHP	C	4	2,3	10,11,12	1.70	3 (30%)	11,14,16	0.90	0
2	GHP	C	5	2	10,11,12	1.96	4 (40%)	11,14,16	1.80	6 (54%)
2	3FG	C	7	2	12,13,13	2.86	8 (66%)	14,18,18	1.38	1 (7%)
2	OMZ	C	2	2	12,14,15	1.47	2 (16%)	17,19,21	1.17	2 (11%)
2	OMY	C	6	2	12,14,15	1.88	4 (33%)	17,19,21	1.62	2 (11%)

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	MLU	C	1	2	-	4/5/8/10	-
2	GHP	C	4	2,3	-	1/4/6/8	0/1/1/1
2	GHP	C	5	2	-	0/4/6/8	0/1/1/1
2	3FG	C	7	2	-	4/8/8/8	0/1/1/1
2	OMZ	C	2	2	-	0/9/10/12	0/1/1/1
2	OMY	C	6	2	-	0/9/10/12	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	3FG	CG1-CB	5.80	1.47	1.39
2	C	7	3FG	CB-CA	4.04	1.57	1.52
2	C	5	GHP	CA-C	3.50	1.56	1.51
2	C	6	OMY	CZ-CE1	3.34	1.42	1.39
2	C	7	3FG	CG2-CD2	3.28	1.44	1.39
2	C	2	OMZ	CD2-CG	3.10	1.44	1.39
2	C	7	3FG	CZ-CD1	3.03	1.43	1.39
2	C	4	GHP	C3-C2	3.01	1.43	1.38
2	C	6	OMY	OCZ-CZ	2.77	1.41	1.36
2	C	7	3FG	OXT-C	-2.60	1.22	1.30
2	C	1	MLU	CA-N	2.52	1.51	1.47
2	C	5	GHP	C1-CA	2.52	1.55	1.52
2	C	6	OMY	CD2-CG	2.40	1.42	1.39
2	C	2	OMZ	CZ-CE1	2.35	1.41	1.39
2	C	4	GHP	O4-C4	2.32	1.42	1.37
2	C	7	3FG	CA-C	2.31	1.60	1.54
2	C	6	OMY	CA-N	-2.31	1.41	1.47
2	C	4	GHP	C3-C4	2.28	1.43	1.39
2	C	7	3FG	CG2-CB	2.28	1.42	1.39
2	C	1	MLU	CB-CA	-2.22	1.51	1.53
2	C	5	GHP	C6-C1	2.21	1.42	1.39
2	C	7	3FG	O-C	2.19	1.28	1.22
2	C	5	GHP	C3-C4	2.07	1.42	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	OMY	CG-CB-CA	-5.43	104.45	111.58
2	C	7	3FG	CB-CA-C	2.97	116.51	110.10
2	C	5	GHP	C2-C1-CA	-2.64	116.53	120.64
2	C	5	GHP	C2-C3-C4	-2.60	117.12	119.88
2	C	2	OMZ	O-C-CA	-2.47	118.42	124.77
2	C	2	OMZ	OC-CB-CG	-2.30	106.21	111.20
2	C	5	GHP	C5-C6-C1	-2.26	118.92	121.18
2	C	5	GHP	C1-CA-C	-2.13	106.11	112.09
2	C	5	GHP	C6-C1-CA	2.13	123.94	120.64
2	C	5	GHP	C3-C2-C1	2.01	123.19	121.18
2	C	6	OMY	OCZ-CZ-CE1	2.00	124.08	119.25

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	MLU	C-CA-CB-CG
2	C	7	3FG	C-CA-CB-CG1
2	C	7	3FG	C-CA-CB-CG2
2	C	7	3FG	O-C-CA-CB
2	C	7	3FG	OXT-C-CA-CB
2	C	1	MLU	N-CA-CB-CG
2	C	1	MLU	CA-CB-CG-CD2
2	C	1	MLU	CA-CB-CG-CD1
2	C	4	GHP	C6-C1-CA-C

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	MLU	2	0
2	C	5	GHP	4	0
2	C	7	3FG	2	0
2	C	6	OMY	2	0

5.5 Carbohydrates [i](#)

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	BGC	D	1	2,3	11,11,12	1.92	2 (18%)	15,15,17	1.75	2 (13%)
3	RER	D	2	3	7,10,11	0.54	0	6,15,17	0.59	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	BGC	D	1	2,3	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RER	D	2	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	BGC	O6-C6	-4.53	1.23	1.42
3	D	1	BGC	C6-C5	-3.04	1.41	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	BGC	O6-C6-C5	5.03	128.46	111.33
3	D	1	BGC	C1-C2-C3	2.81	113.73	109.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

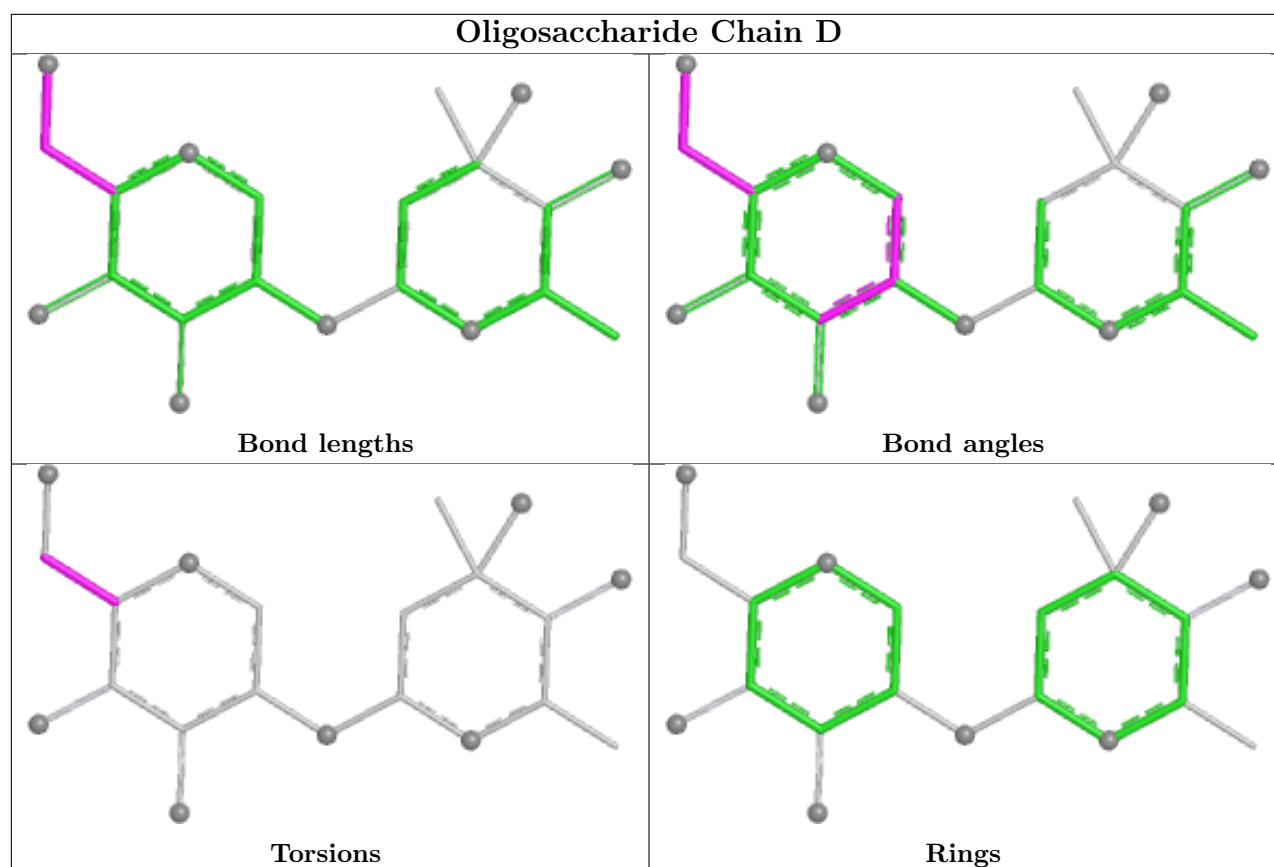
Mol	Chain	Res	Type	Atoms
3	D	1	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	RER	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](#)

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	$\# Z > 2$
4	TYD	A	405	-	25,26,26	0.86	1 (4%)	38,40,40	0.70	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
4	TYD	A	405	-	-	0/16/28/28	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	TYD	PA-O3A	3.64	1.63	1.59

There are no bond angle outliers.

There are no chirality outliers.

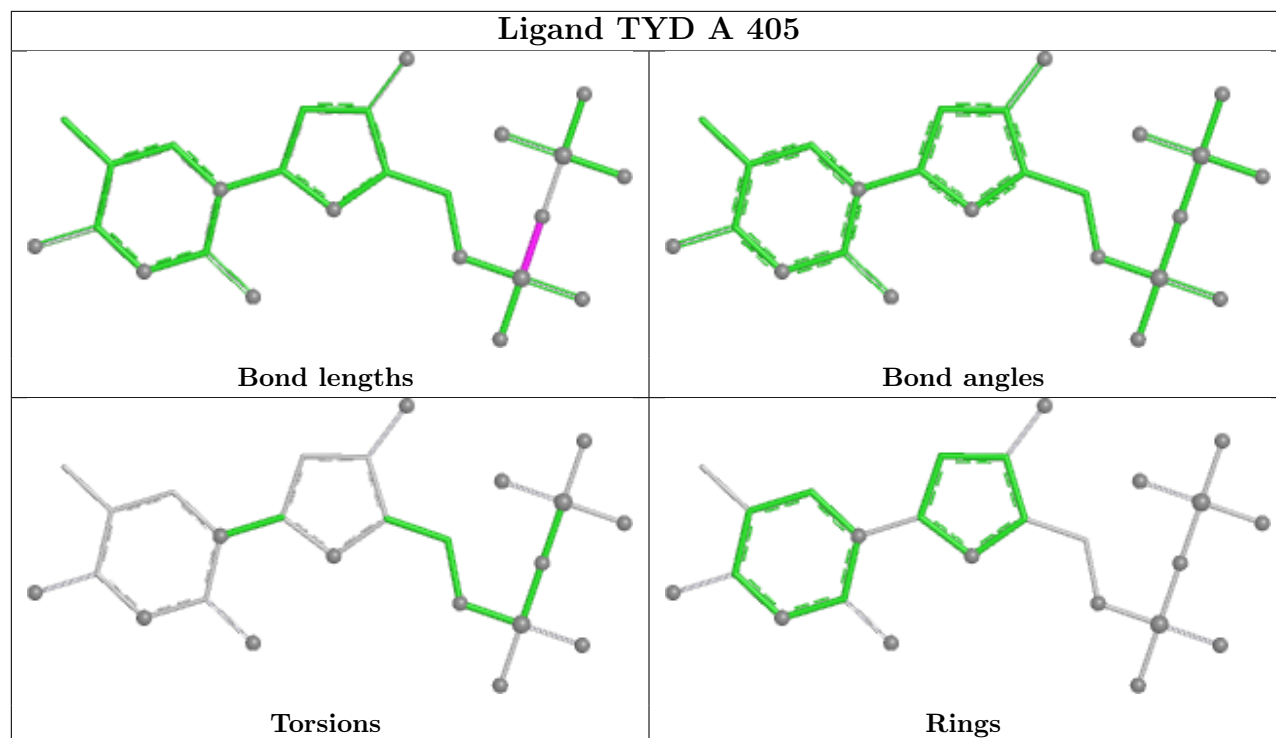
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	TYD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	382/404 (94%)	0.25	11 (2%) 53 43	36, 63, 88, 97	1 (0%)
1	B	384/404 (95%)	0.22	11 (2%) 53 43	37, 59, 76, 99	0
2	C	1/7 (14%)	1.32	0 100 100	49, 49, 49, 49	0
All	All	767/815 (94%)	0.24	22 (2%) 53 43	36, 61, 85, 99	1 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	GLU	4.4
1	B	391	LYS	3.5
1	A	315	VAL	3.4
1	B	323	ALA	3.4
1	B	324	TYR	3.4
1	A	175	ASP	3.1
1	B	315	VAL	3.0
1	B	127	ASP	3.0
1	B	134	SER	2.9
1	A	13	ASP	2.7
1	A	65	GLY	2.6
1	B	265	LEU	2.4
1	A	390	GLU	2.4
1	B	29	ALA	2.3
1	B	28	GLY	2.3
1	B	193	LEU	2.2
1	A	193	LEU	2.2
1	B	267	ASP	2.1
1	A	67	LEU	2.1
1	A	194	GLY	2.1
1	A	221	SER	2.1
1	A	143	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

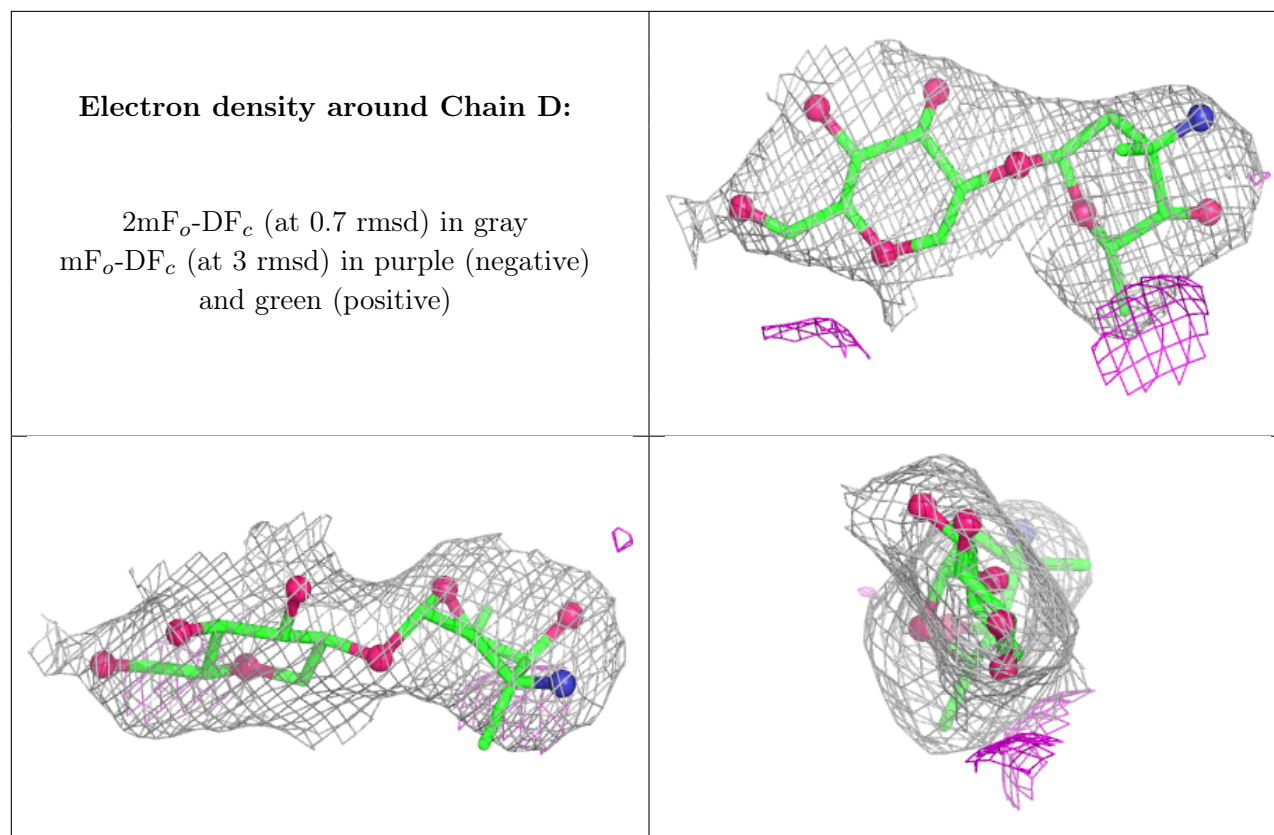
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OMZ	C	2	14/15	0.54	0.20	52,53,57,58	0
2	OMY	C	6	14/15	0.55	0.20	48,50,57,59	0
2	MLU	C	1	9/10	0.92	0.13	52,53,56,56	0
2	3FG	C	7	13/13	0.93	0.10	49,52,62,62	0
2	GHP	C	4	11/12	0.94	0.09	45,50,53,55	0
2	GHP	C	5	11/12	0.95	0.11	50,51,53,55	0

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	D	1	11/12	0.95	0.07	56,59,63,63	0
3	RER	D	2	10/11	0.95	0.09	55,58,58,59	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

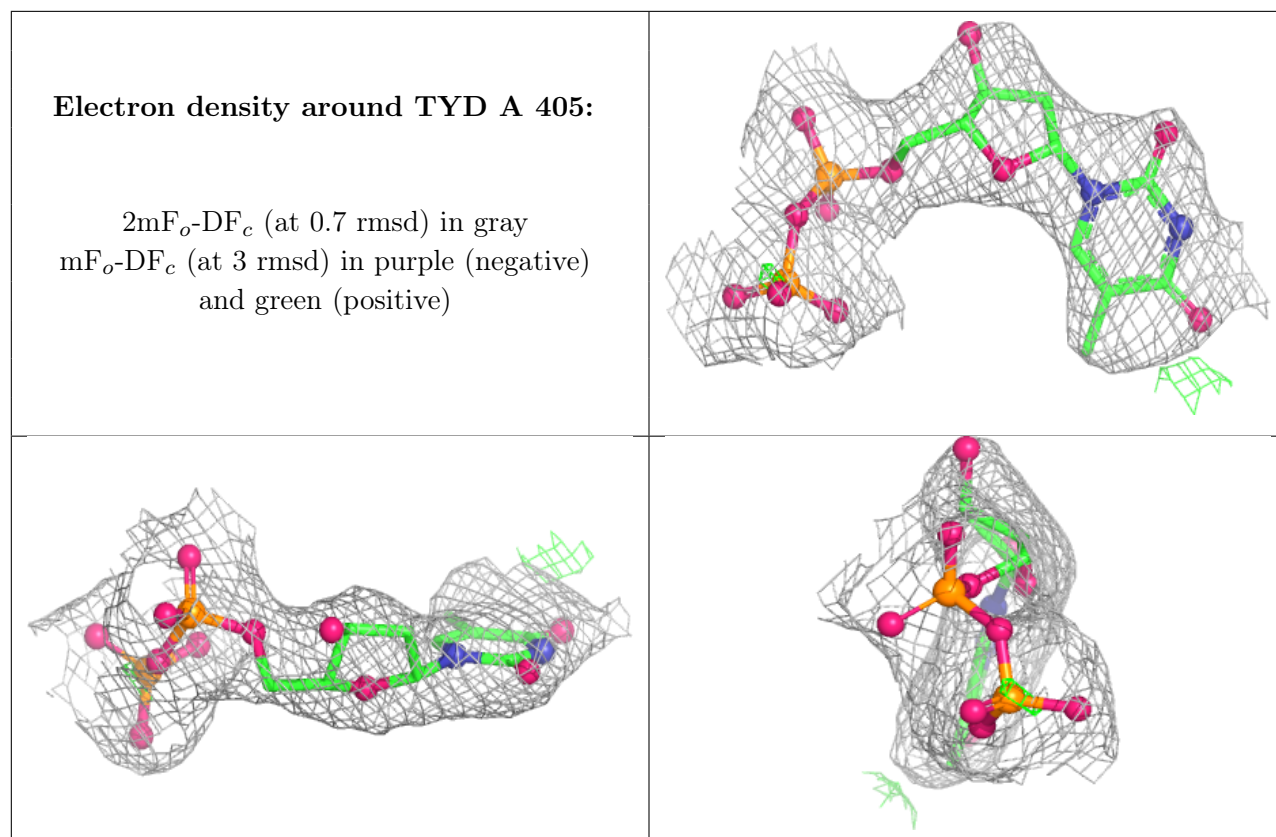


6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TYD	A	405	25/25	0.96	0.10	66,74,77,78	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.