Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 03:39 PM EDT

PDB ID	:	1PNV
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:

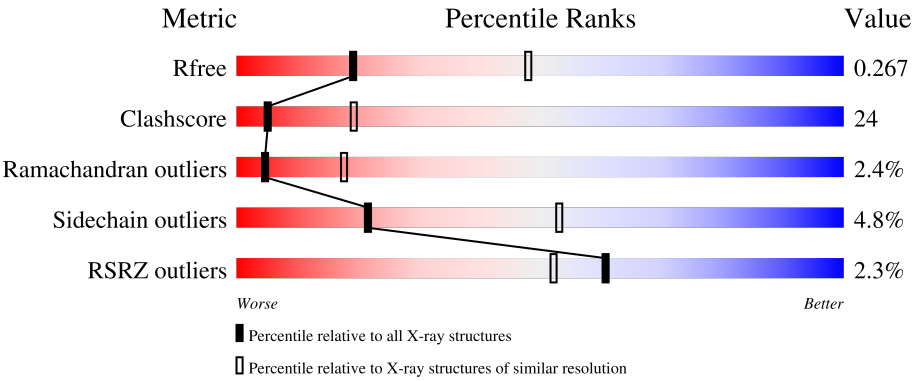
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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 <=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	2% 57% 33% · 5%
1	B	404	3% 58% 34% · 5%
2	C	7	14% 29% 57%
3	D	2	100%

2 Entry composition (i)

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			

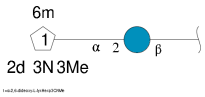
There are 16 discrepancies between the modelled and reference sequences:

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.

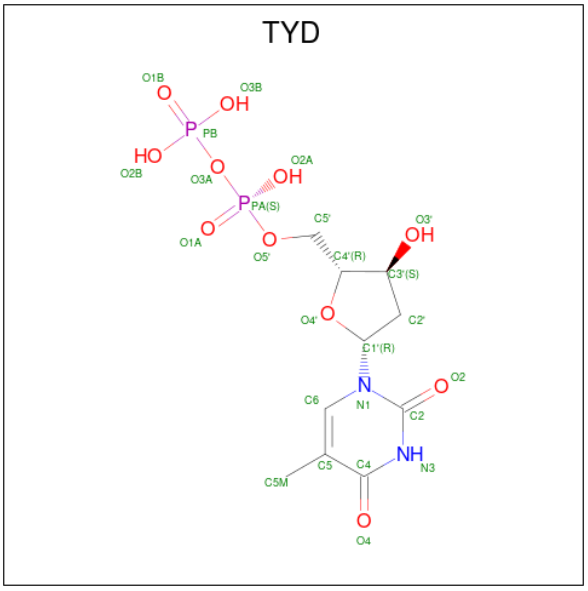
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	Cl	N	O	0	0	0
			80	53	2	8	17			

- 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 21 13 1 7	0	0	0

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



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

- Molecule 5 is water.

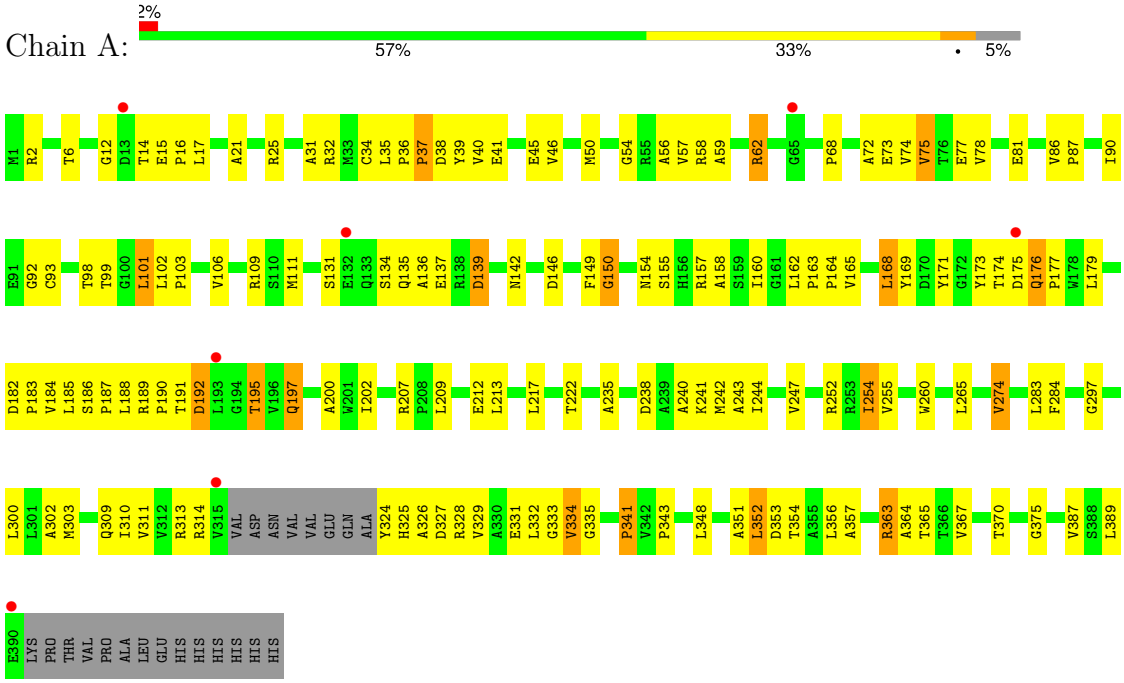
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	43	Total O 43 43	0	0
5	C	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

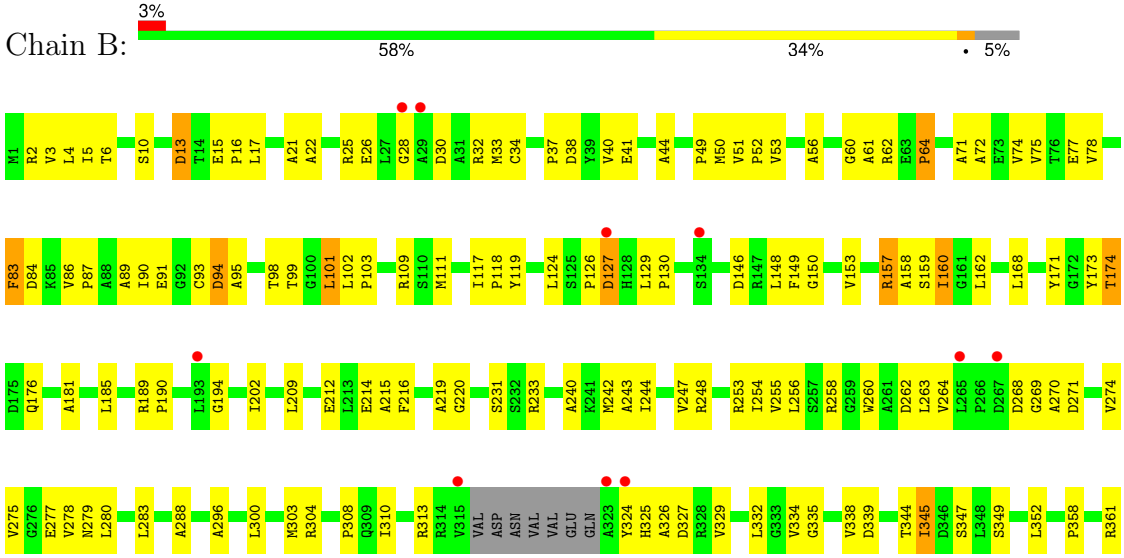
• Molecule 1: GLYCOSYLTRANSFERASE GTFA

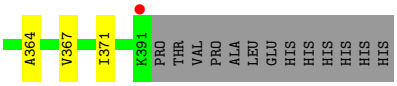
Chain A:



• Molecule 1: GLYCOSYLTRANSFERASE GTFA

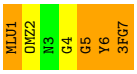
Chain B:





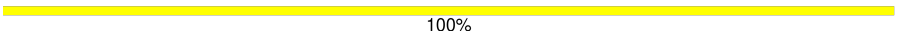
• Molecule 2: VANCOMYCIN

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.57 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.269 0.225 , 0.267	Depositor DCC
R_{free} test set	1489 reflections (4.39%)	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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: RER, OMY, BGC, MLU, 3FG, OMZ, TYD, GHP

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	0.35	0/2843	0.64	0/3894
1	B	0.37	0/2839	0.64	0/3891
2	C	0.95	0/7	1.21	0/8
All	All	0.36	0/5689	0.64	0/7793

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	2787	0	2763	144	0
1	B	2784	0	2742	128	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	273	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 24.

All (273) 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: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: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: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
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: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:252:ARG:CZ	1:A:356:LEU:HD13	2.18	0.74
1:B:86:VAL:HB	1:B:111:MET:HE3	1.69	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:A:87:PRO:HD3	1:A:111:MET:HE3	1.71	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:87:PRO:HD3	1:A:111:MET:CE	2.29	0.62
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:A:134:SER:C	1:A:136:ALA:H	2.04	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:40:VAL:HA	1:B:50:MET:HE3	1.84	0.59
1:B:202:ILE:HD12	1:B:304:ARG:CZ	2.33	0.59
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:84:ASP:O	1:B:87:PRO:HD2	2.04	0.57
1:A:244:ILE:HD12	1:A:254:ILE:HD11	1.86	0.57
1:A:185:LEU:HD13	1:A:303:MET:CE	2.34	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:269:GLY:C	1:B:271:ASP:H	2.13	0.53
1:A:313:ARG:HG3	1:A:314:ARG:H	1.73	0.53
1:B:303:MET:HE3	1:B:332:LEU:HD13	1.90	0.53
1:A:149:PHE:CD1	1:A:168:LEU:HD23	2.44	0.53
1:B:310:ILE:HD11	1:B:352:LEU:HA	1.90	0.53
1:B:158:ALA:C	1:B:160:ILE:H	2.13	0.52
1:B:87:PRO:HD3	1:B:111:MET:HE3	1.90	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:363:ARG:O	1:A:363:ARG:HG3	2.13	0.49
1:B:86:VAL:HB	1:B:111:MET:CE	2.39	0.48
1:B:83:PHE:O	1:B:111:MET:HE1	2.12	0.48
2:C:5:GHP:C2	2:C:7:3FG:HN1	2.26	0.48
1:A:185:LEU:HD13	1:A:303:MET:HE1	1.95	0.48
1:B:329:VAL:CG1	1:B:335:GLY:HA3	2.43	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:B:60:GLY:C	1:B:62:ARG:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:CG2	1:B:176:GLN:H	2.28	0.47
1:B:334:VAL:HG21	1:B:367:VAL:HG21	1.97	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
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: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: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: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: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: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:B:339:ASP:OD2	1:B:339:ASP:C	2.54	0.45
1:A:184:VAL:HG21	1:A:370:THR:OG1	2.17	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:51:VAL:HG13	1:B:51:VAL:O	2.17	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
1:B:303:MET:CE	1:B:371:ILE:HD11	2.47	0.44
1:B:255:VAL:HG11	1:B:283:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:SER:C	1:A:136:ALA:N	2.71	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: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:A:14:THR:C	1:A:16:PRO:HD2	2.40	0.42
1:B:248:ARG:NH1	1:B:271:ASP:OD2	2.52	0.42
1:A:165:VAL:HG23	1:A:168:LEU:HD11	2.01	0.42
1:A:185:LEU:HD13	1:A:303:MET:HE3	2.00	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:3:VAL:HG13	1:B:95:ALA:HB3	2.00	0.42
1:A:351:ALA:C	1:A:353:ASP:N	2.73	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:A:149:PHE:O	1:A:150:GLY:C	2.58	0.42
1:B:5:ILE:HD12	1:B:21:ALA:HB2	2.02	0.42
1:A:189:ARG:C	1:A:191:THR:H	2.23	0.41
1:B:220:GLY:C	1:B:253:ARG:NH1	2.73	0.41
1:B:269:GLY:C	1:B:271:ASP:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:O	1:A:75:VAL:C	2.58	0.41
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:280:LEU:HA	1:B:280:LEU:HD12	1.82	0.41
1:B:303:MET:HE3	1:B:332:LEU:CD1	2.51	0.41
1:A:21:ALA:O	1:A:25:ARG:HG3	2.21	0.41
1:A:35:LEU:HB2	1:A:50:MET:HE2	2.02	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:B:325:HIS:O	1:B:326:ALA:C	2.60	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:B:268:ASP:O	1:B:269:GLY:C	2.59	0.41
1:A:387:VAL:CG1	1:B:264:VAL:HG22	2.51	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 (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	378/404 (94%)	343 (91%)	27 (7%)	8 (2%)	5 20
1	B	380/404 (94%)	353 (93%)	17 (4%)	10 (3%)	4 16
2	C	1/7 (14%)	1 (100%)	0	0	100 100
All	All	759/815 (93%)	697 (92%)	44 (6%)	18 (2%)	5 18

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 (i)

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%)	264 (94%)	16 (6%)	17 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	278/311 (89%)	267 (96%)	11 (4%)	27 60
2	C	1/1 (100%)	1 (100%)	0	100 100
All	All	559/623 (90%)	532 (95%)	27 (5%)	21 53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	62	ARG
1	A	73	GLU
1	A	139	ASP
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	13	ASP
1	B	64	PRO
1	B	77	GLU
1	B	83	PHE
1	B	94	ASP
1	B	119	TYR
1	B	127	ASP
1	B	157	ARG
1	B	174	THR
1	B	338	VAL
1	B	345	ILE

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	OMY	C	6	2	12,14,15	1.88	4 (33%)	17,19,21	1.62	2 (11%)
2	GHP	C	5	2	10,11,12	1.96	4 (40%)	11,14,16	1.80	6 (54%)
2	OMZ	C	2	2	12,14,15	1.47	2 (16%)	17,19,21	1.17	2 (11%)
2	3FG	C	7	2	12,13,13	2.86	8 (66%)	14,18,18	1.38	1 (7%)
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

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	OMY	C	6	2	-	0/9/10/12	0/1/1/1
2	GHP	C	5	2	-	0/4/6/8	0/1/1/1
2	OMZ	C	2	2	-	0/9/10/12	0/1/1/1
2	3FG	C	7	2	-	4/8/8/8	0/1/1/1
2	MLU	C	1	2	-	4/5/8/10	-
2	GHP	C	4	2,3	-	1/4/6/8	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(^{o})	Ideal(^{o})
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	6	OMY	2	0
2	C	5	GHP	4	0
2	C	7	3FG	2	0
2	C	1	MLU	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

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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(^{o})	Ideal(^{o})
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:

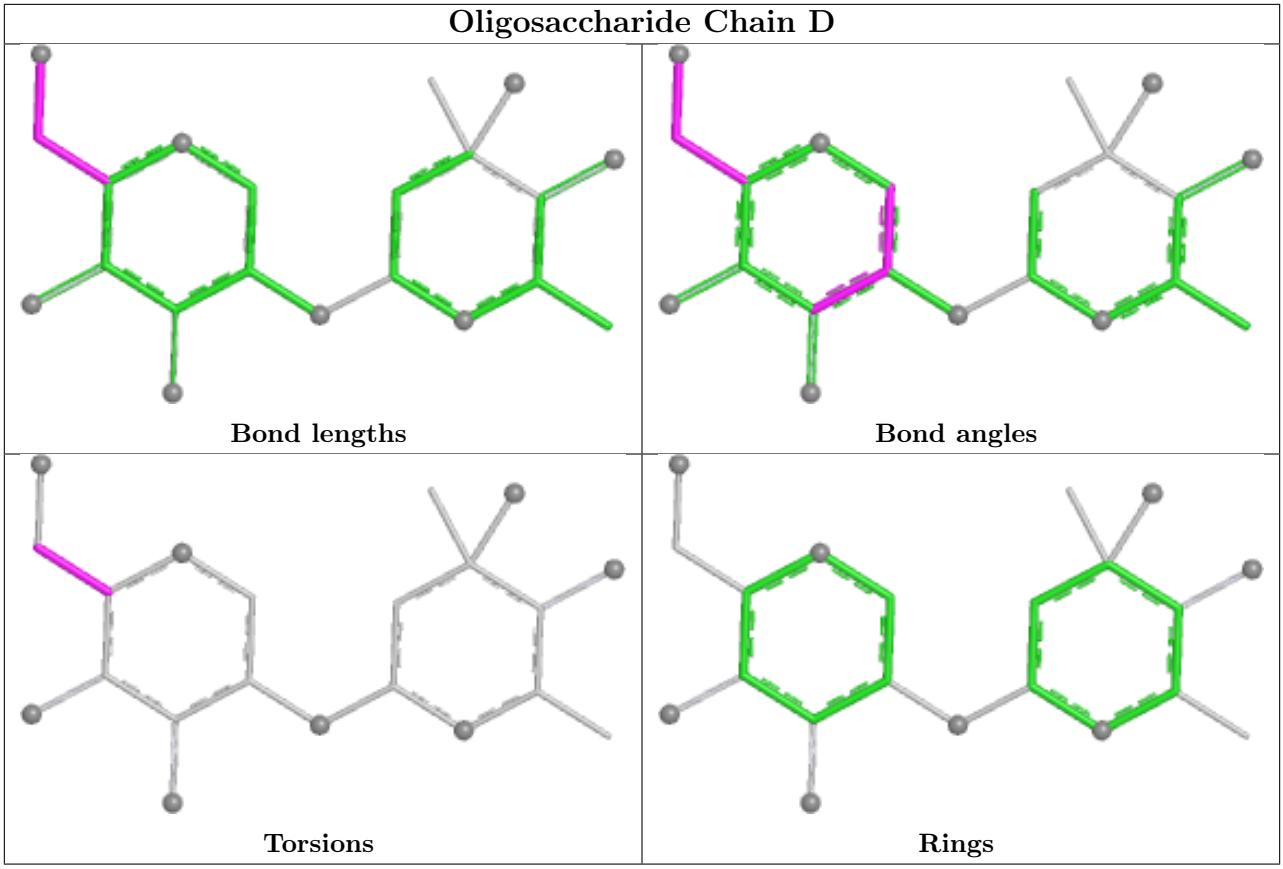
Mol	Chain	Res	Type	Atoms
3	D	1	BGC	O5-C5-C6-O6

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	-	22,26,26	1.38	3 (13%)	29,40,40	2.87	2 (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
4	TYD	A	405	-	-	0/13/28/28	0/2/2/2

All (3) 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
4	A	405	TYD	C6-N1	3.15	1.38	1.33
4	A	405	TYD	C4-N3	3.13	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	405	TYD	C2-N3-C4	14.47	127.31	115.09
4	A	405	TYD	C6-N1-C2	2.20	120.98	119.10

There are no chirality outliers.

There are no torsion outliers.

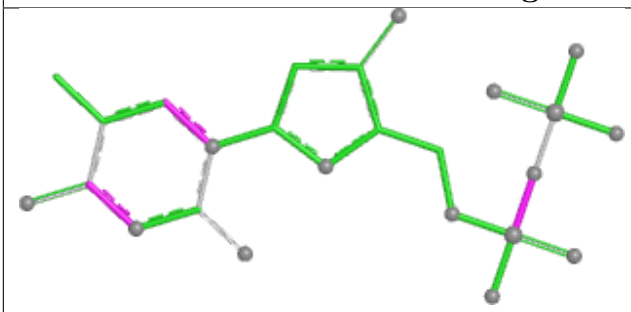
There are no ring outliers.

1 monomer is involved in 4 short contacts:

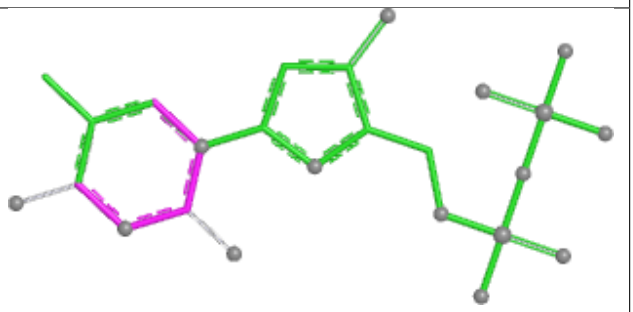
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	TYD	4	0

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 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.

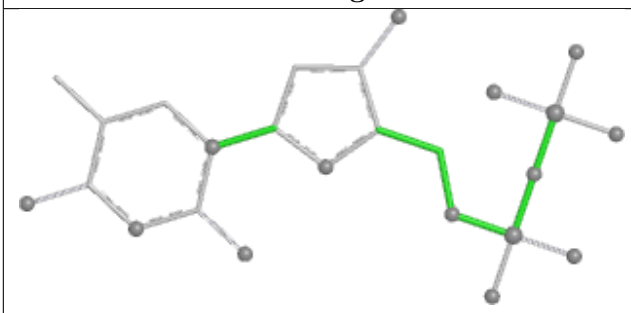
Ligand TYD A 405



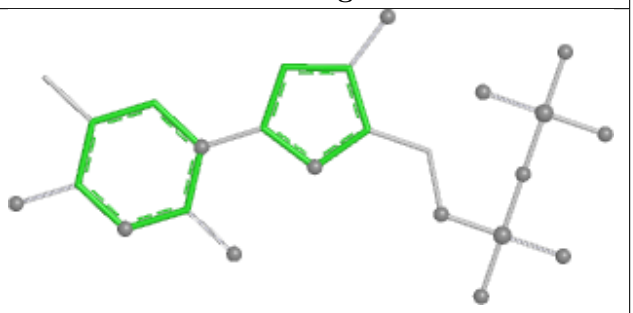
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.11	7 (1%) 67 60	36, 63, 88, 97	1 (0%)
1	B	384/404 (95%)	0.08	11 (2%) 54 45	37, 59, 76, 99	0
2	C	1/7 (14%)	1.19	0 100 100	49, 49, 49, 49	0
All	All	767/815 (94%)	0.09	18 (2%) 61 52	36, 61, 85, 99	1 (0%)

All (18) 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	3.3
1	B	323	ALA	3.3
1	B	324	TYR	3.2
1	A	175	ASP	3.0
1	B	315	VAL	3.0
1	B	127	ASP	2.9
1	B	134	SER	2.8
1	A	13	ASP	2.6
1	A	65	GLY	2.5
1	A	390	GLU	2.3
1	B	265	LEU	2.3
1	B	29	ALA	2.2
1	B	28	GLY	2.1
1	B	193	LEU	2.1
1	A	193	LEU	2.0
1	B	267	ASP	2.0

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, 95^{th} 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)

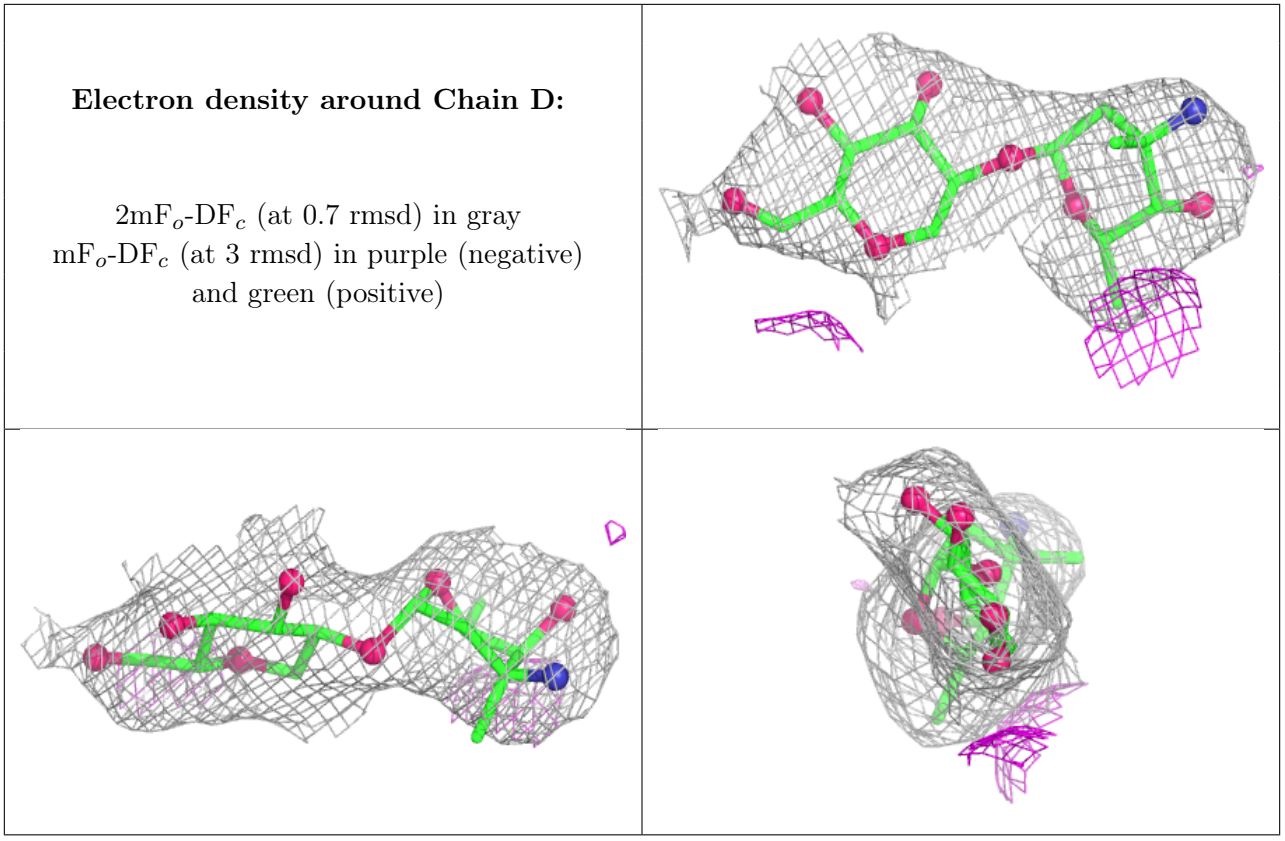
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

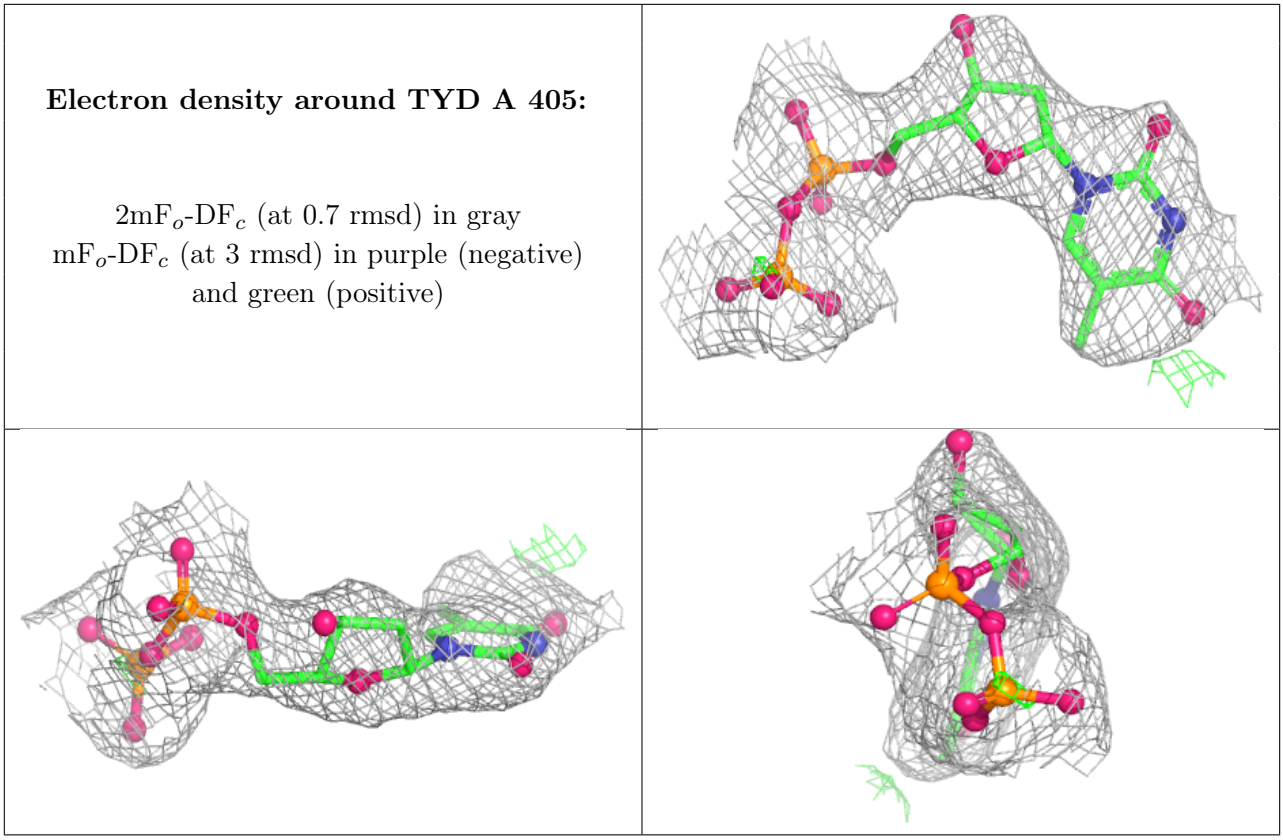
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Electron density around TYD A 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.