Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:34 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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	Percentile Ranks	Value
Rfree		0.268
Clashscore		24
Ramachandran outliers		2.4%
Sidechain outliers		4.8%
RSRZ outliers		1.8%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
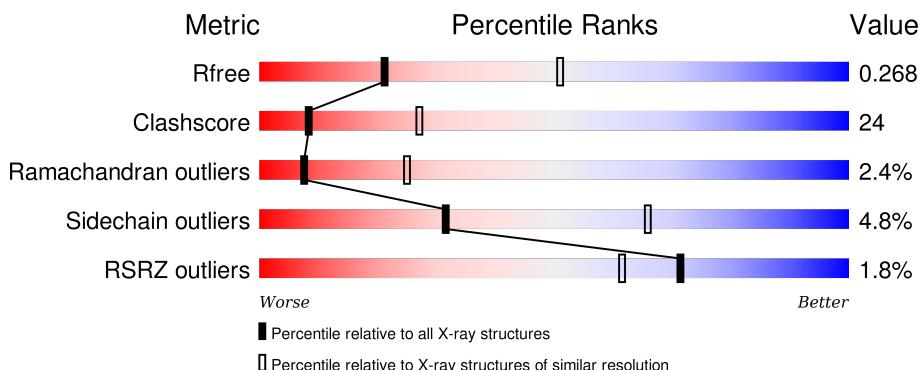
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	% — 58% / 34% / • 5%
2	C	7	43% / 57%
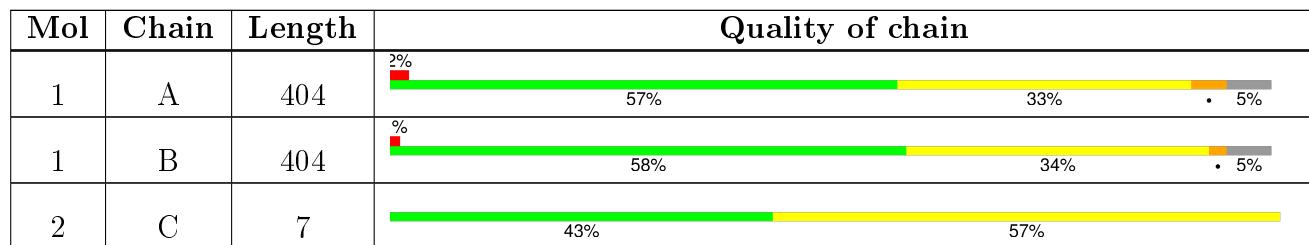
2 Entry composition ⓘ

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 2787	C 1757	N 490	O 528	S 12	0	0	0
1	B	384	Total 2784	C 1749	N 493	O 530	S 12	0	0	0

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 80	C 53	Cl 2	N 8	O 17	0	0	0

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula:

$C_{10}H_{16}N_2O_{11}P_2$).
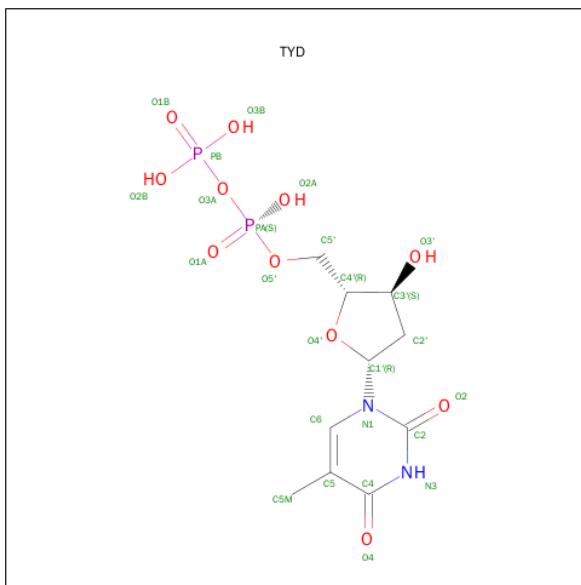
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
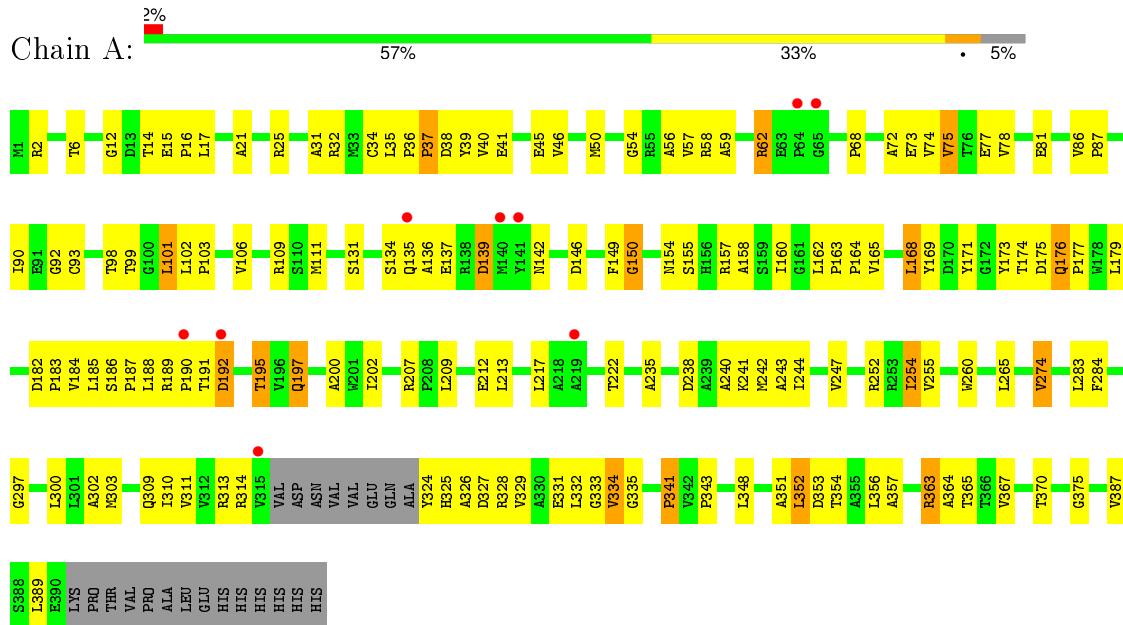
- Molecule 1: GLYCOSYLTRANSFERASE GTFA
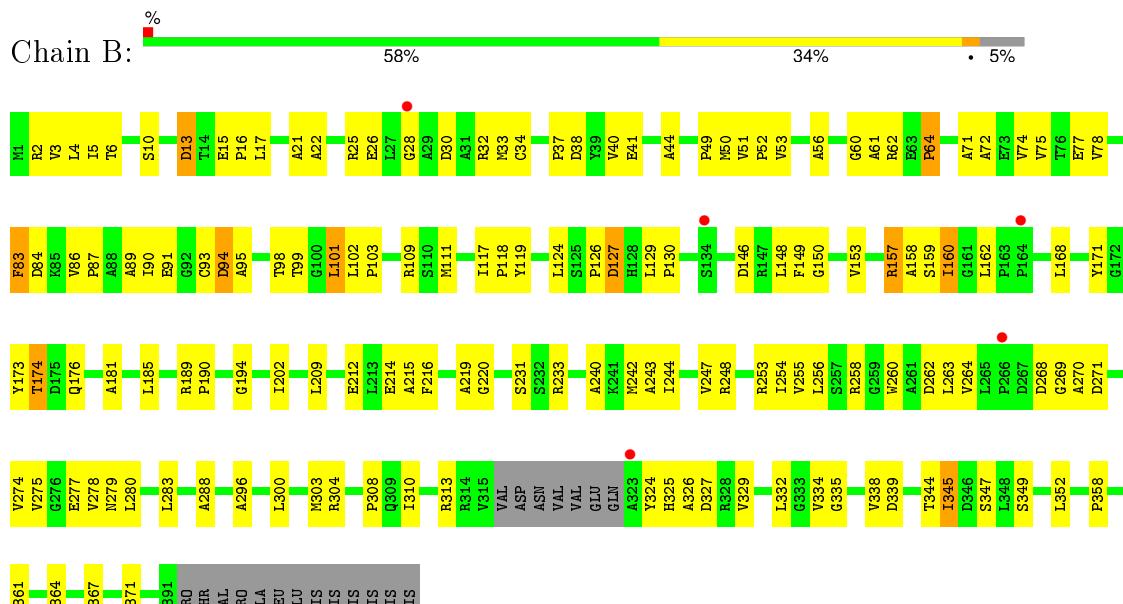
● Molecule 2: VANCOMYCIN

Chain C:
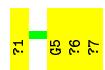
4 Data and refinement statistics (i)

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 29.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.80) 94.0 (29.94-2.70)	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 0.226 , 0.268	Depositor DCC
R_{free} test set	1405 reflections (4.39%)	DCC
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 , 53.5	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 37562 reflections (0.003%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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 (i)

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	A	25	0	13	4	0
4	C	21	0	21	1	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:17:LEU:HD11	1:A:99:THR:HG22	1.74	0.69
1:A:6:THR:CG2	1:A:34:CYS:HB2	2.22	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:N	1:B:345:ILE:HD12	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

Continued on next page...

Continued from previous page...

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:HG2	1:A:2:ARG:HH11	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	3: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:244:ILE:HG23	1:A:254:ILE:HD13	1.86	0.56
1:A:185:LEU:HD13	1:A:303:MET:CE	2.34	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:B:345:ILE:O	1:B:349:SER:HB2	2.06	0.56
1:A:175:ASP:O	1:A:176:GLN:HG2	2.05	0.56
1:B:51:VAL:HG11	1:B:89:ALA:HB2	1.88	0.56
1:A:45:GLU:OE1	1:A:207:ARG:HD3	2.06	0.56
1:A:54:GLY:HA2	1:A:81:GLU:OE1	2.06	0.56

Continued on next page...

Continued from previous page...

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:B:244:ILE:HD11	1:B:256:LEU:HD13	1.88	0.54
1:A:300:LEU:HD12	5:A:2013:HOH:O	2.07	0.54
1:A:187:PRO:HG2	5:A:2014:HOH:O	2.08	0.54
2:C:6:OMY:CL	4:C:9: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:389:LEU:HD21	1:B:212:GLU:CG	2.33	0.53
1:A:15:GLU:N	1:A:16:PRO:HD2	2.23	0.53
1:B:269:GLY:C	1:B:271:ASP:H	2.13	0.53
1:B:303:MET:HE3	1:B:332:LEU:HD13	1.90	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: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:188:LEU:HD22	1:A:192:ASP:OD2	2.10	0.52
1:A:179:LEU:CD2	1:A:197:GLN:NE2	2.71	0.52
1:B:174:THR:HG22	1:B:176:GLN:N	2.25	0.52
1:A:87:PRO:HA	1:A:90:ILE:HG22	1.91	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:B:243:ALA:O	1:B:247:VAL:HG23	2.10	0.51
1:B:158:ALA:O	1:B:160:ILE:N	2.43	0.51
1:B:258:ARG:NH1	1:B:262:ASP:HB3	2.26	0.51
1:A:200:ALA:O	1:A:375:GLY:HA3	2.11	0.51
1:A:98:THR:CG2	1:A:99:THR:N	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HH21	1:A:162:LEU:HD22	1.75	0.51
1:A:74:VAL:O	1:A:77:GLU:N	2.41	0.51
1:B:40:VAL:HG23	1:B:41:GLU:N	2.25	0.51
1:A:235:ALA:CB	1:A:341:PRO:HB2	2.41	0.51
1:A:235:ALA:HB1	1:A:341:PRO:HB2	1.93	0.51
1:A:12:GLY:HA2	3:A:405:TYD:C5'	2.41	0.51
1:A:334:VAL:HG12	1:A:364:ALA:HA	1.92	0.50
1:A:202:ILE:HD11	1:A:300:LEU:HD21	1.93	0.50
1:A:142:ASN:OD1	1:A:169:TYR:HB3	2.11	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:NH1	1:A:2:ARG:HG2	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:94:ASP:O	1:B:118:PRO:HD2	2.11	0.49
1:A:106:VAL:HG13	1:A:171:TYR:HD2	1.77	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:B:13:ASP:HA	1:B:124:LEU:CD1	2.43	0.49
1:A:150:GLY:O	1:A:154:ASN:ND2	2.40	0.49
1:A:56:ALA:HB3	1:A:62:ARG:HG3	1.95	0.49
1:A:154:ASN:H	1:A:154:ASN:ND2	2.11	0.49
1:A:363:ARG:HG3	1:A:363:ARG:O	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	3: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:N	1:B:127:ASP:OD1	2.46	0.47
1:B:98:THR:HG22	1:B:99:THR:N	2.29	0.47
1:B:4:LEU:HD22	1:B:90:ILE:HB	1.95	0.47
1:A:176:GLN:NE2	1:A:195:THR:HG22	2.29	0.47

Continued on next page...

Continued from previous page...

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:309:GLN:O	1:A:335:GLY:HA3	2.16	0.46
1:A:146:ASP:O	1:A:150: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:325:HIS:O	1:A:329:VAL:HG23	2.15	0.46
1:A:59:ALA:HA	1:A:62:ARG:NH2	2.31	0.46
1:A:154:ASN:HA	1:A:157:ARG:HB2	1.97	0.46
1:A:2:ARG:HD2	1:A:92:GLY:O	2.15	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:101:LEU:HD13	2:C:5:GHP:C6	2.46	0.45
1:B:32:ARG:HD3	1:B:49:PRO:CG	2.46	0.45
1:A:75:VAL:HG12	1:A:149:PHE:HB3	1.98	0.45
1:B:86:VAL:HG11	1:B:111:MET:HG3	1.99	0.45
1:A:72:ALA:O	1:A:75:VAL:HG23	2.16	0.45
1:B:109:ARG:HD3	1:B:171:TYR:CZ	2.51	0.45
2:C:5:GHP:C2	2:C:7:3FG:N	2.80	0.45
1:A:324:TYR:O	1:A:328:ARG:HG2	2.17	0.45
1:B:339:ASP:C	1:B:339:ASP:OD2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:CA	3: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:46:VAL:O	1:A:46:VAL:HG12	2.17	0.44
1:A:244:ILE:CD1	1:A:254:ILE:CD1	2.94	0.44
1:A:134:SER:C	1:A:136:ALA:N	2.71	0.44
1:B:52:PRO:O	1:B:53:VAL:CG2	2.66	0.44
1:B:260:TRP:HZ2	1:B:277:GLU:CG	2.25	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: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:N	1:A:139:ASP:OD1	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:309:GLN:HG3	1:A:329:VAL:HG11	2.00	0.43
1:A:241:LYS:HE3	5:A:2020:HOH:O	2.19	0.43
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:155:SER:O	1:A:158:ALA:HB3	2.18	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:14:THR:C	1:A:16:PRO:HD2	2.40	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:B:160:ILE:HG12	1:B:160:ILE:O	2.20	0.42
1:A:351:ALA:C	1:A:353:ASP:N	2.73	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: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
1:A:189:ARG:C	1:A:191:THR:H	2.23	0.41

Continued on next page...

Continued from previous page...

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:185:LEU:HD21	1:B:325:HIS:HD2	1.85	0.41
1:B:37:PRO:HG2	1:B:56:ALA:HB2	2.01	0.41
1:B:258:ARG:HG3	1:B:274:VAL:HG13	2.02	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:A:102:LEU:N	1:A:103:PRO:HD2	2.35	0.41
1:B:303:MET:HE3	1:B:332:LEU:CD1	2.51	0.41
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.82	0.41
1:A:150:GLY:HA2	1:A:168:LEU:CD2	2.51	0.41
1:A:72:ALA:HA	1:A:75:VAL:CG2	2.51	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:354:THR:O	1:A:357:ALA:HB3	2.21	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: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:62:ARG:NH1	1:A:68:PRO:N	2.69	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:HA	2:C:1:MLU:HD23	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%)	9	29
1	B	380/404 (94%)	353 (93%)	17 (4%)	10 (3%)	7	22
2	C	1/7 (14%)	1 (100%)	0	0	100	100
All	All	759/815 (93%)	697 (92%)	44 (6%)	18 (2%)	7	25

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%)	25	58

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	278/311 (89%)	267 (96%)	11 (4%)	38	73
2	C	1/1 (100%)	1 (100%)	0	100	100
All	All	559/623 (90%)	532 (95%)	27 (5%)	31	66

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

Some 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	A	197	GLN
1	B	176	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	1.22	1 (14%)	4,9,11	1.01	0
2	OMZ	C	2	2	13,14,15	1.68	3 (23%)	17,19,21	1.25	3 (17%)
2	GHP	C	4	2,4	10,11,12	1.58	3 (30%)	12,14,16	0.95	0
2	GHP	C	5	2	10,11,12	1.74	3 (30%)	12,14,16	2.17	5 (41%)
2	OMY	C	6	2	13,14,15	1.97	4 (30%)	17,19,21	1.56	1 (5%)
2	3FG	C	7	2	9,13,13	2.93	5 (55%)	14,18,18	1.52	2 (14%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	7	3FG	CG2-CB	2.07	1.42	1.39
2	C	4	GHP	O4-C4	2.13	1.42	1.37
2	C	4	GHP	C3-C4	2.16	1.43	1.38
2	C	5	GHP	CA-C	2.17	1.56	1.50
2	C	5	GHP	C6-C1	2.19	1.42	1.39
2	C	1	MLU	CA-N	2.37	1.51	1.47
2	C	6	OMY	CD2-CG	2.37	1.42	1.39
2	C	2	OMZ	CZ-CE1	2.45	1.41	1.39
2	C	6	OMY	OCZ-CZ	2.65	1.41	1.36
2	C	4	GHP	C3-C2	2.74	1.43	1.38
2	C	5	GHP	C1-CA	2.75	1.55	1.52
2	C	7	3FG	CZ-CD1	2.88	1.43	1.39
2	C	2	OMZ	CD2-CG	3.04	1.44	1.39
2	C	7	3FG	CG2-CD2	3.11	1.44	1.39
2	C	6	OMY	CA-CB	3.30	1.60	1.54
2	C	6	OMY	CZ-CE1	3.44	1.42	1.39
2	C	2	OMZ	CA-CB	3.47	1.60	1.54
2	C	7	3FG	CB-CA	4.72	1.57	1.52
2	C	7	3FG	CG1-CB	5.17	1.47	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	-5.37	104.45	111.96
2	C	2	OMZ	O-C-CA	-2.66	118.42	125.44
2	C	5	GHP	C2-C1-CA	-2.42	116.53	120.70
2	C	5	GHP	C2-C3-C4	-2.37	117.12	119.87
2	C	2	OMZ	OC-CB-CG	-2.24	106.21	111.16
2	C	5	GHP	C5-C6-C1	-2.22	118.92	121.20
2	C	5	GHP	C-CA-N	-2.00	104.78	109.12
2	C	2	OMZ	C-CA-N	2.13	114.29	109.83
2	C	7	3FG	CG2-CB-CA	2.14	122.10	119.35
2	C	7	3FG	C-CA-CB	3.82	116.51	111.31
2	C	5	GHP	C1-CA-N	5.03	124.40	112.54

There are no chirality outliers.

There are no torsion outliers.

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	6	OMY	2	0
2	C	7	3FG	2	0

5.5 Carbohydrates (i)

2 carbohydrates 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	$\#|Z| > 2$
4	BGC	C	8	2,4	11,11,12	1.86	2 (18%)	14,15,17	1.93	2 (14%)
4	RER	C	9	4	8,10,11	0.64	0	7,15,17	0.87	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	BGC	C	8	2,4	-	0/2/19/22	0/1/1/1
4	RER	C	9	4	-	0/0/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8	BGC	O6-C6	-4.39	1.23	1.42
4	C	8	BGC	C6-C5	-2.90	1.41	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	8	BGC	C1-C2-C3	3.54	113.73	109.54
4	C	8	BGC	O6-C6-C5	5.18	128.46	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	9	RER	1	0

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	#$|Z| > 2$
3	TYD	A	405	-	19,26,26	1.09	2 (10%)	27,40,40	3.33	4 (14%)

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	TYD	A	405	-	-	0/12/28/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	TYD	C6-N1	2.44	1.38	1.35
3	A	405	TYD	C4-N3	2.83	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	TYD	C5-C4-N3	-8.83	115.30	125.14
3	A	405	TYD	C5M-C5-C6	2.21	123.06	118.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	405	TYD	O3A-PA-O5'	2.65	109.96	102.94
3	A	405	TYD	C4-N3-C2	13.96	127.31	115.25

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
3	A	405	TYD	4	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.05	9 (2%)	62	50	36, 63, 88, 97	1 (0%)
1	B	384/404 (95%)	-0.15	5 (1%)	79	71	37, 59, 76, 99	0
2	C	1/7 (14%)	0.47	0	100	100	49, 49, 49, 49	0
All	All	767/815 (94%)	-0.10	14 (1%)	71	61	36, 61, 85, 99	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	5.5
1	A	315	VAL	4.2
1	B	134	SER	4.1
1	A	64	PRO	3.9
1	B	28	GLY	3.4
1	B	323	ALA	2.6
1	A	141	TYR	2.6
1	A	190	PRO	2.5
1	A	135	GLN	2.4
1	B	266	PRO	2.4
1	A	140	MET	2.4
1	B	164	PRO	2.2
1	A	219	ALA	2.1
1	A	192	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
2	GHP	C	4	11/12	0.95	0.20	-	45,50,53,55	0
2	MLU	C	1	9/10	0.95	0.18	-	52,53,56,56	0
2	GHP	C	5	11/12	0.96	0.20	-	50,51,53,55	0
2	3FG	C	7	13/13	0.96	0.19	-	49,52,62,62	0
2	OMY	C	6	14/15	0.75	0.25	-	48,50,57,59	0
2	OMZ	C	2	14/15	0.73	0.23	-	52,53,57,58	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
4	BGC	C	8	11/12	0.97	0.12	-1.31	56,59,63,63	0
4	RER	C	9	10/11	0.97	0.13	-	55,58,58,59	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
3	TYD	A	405	25/25	0.96	0.20	0.53	66,74,77,78	0

6.5 Other polymers (i)

There are no such residues in this entry.