



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 AM UTC

PDB ID : 2P6P / pdb_00002p6p
Title : X-ray crystal structure of C-C bond-forming dTDP-D-Olivose-transferase UrdGT2
Authors : Mittler, M.; Bechthold, A.; Schulz, G.E.
Deposited on : 2007-03-19
Resolution : 1.88 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
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

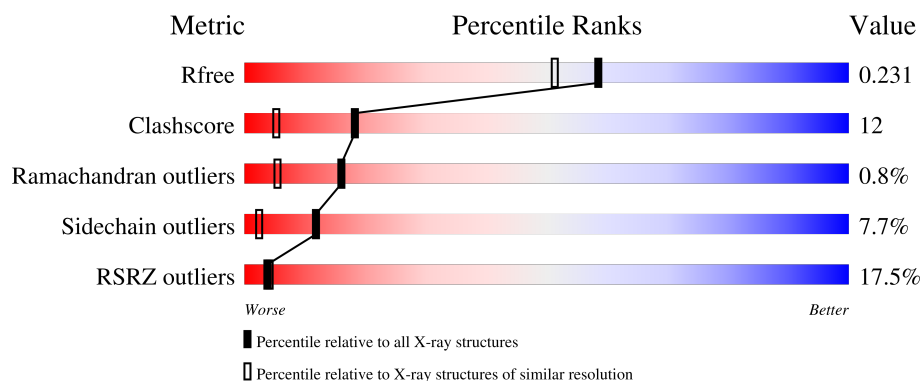
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	384	13% 76% 20% ...
1	B	384	22% 72% 22% ...

2 Entry composition [i](#)

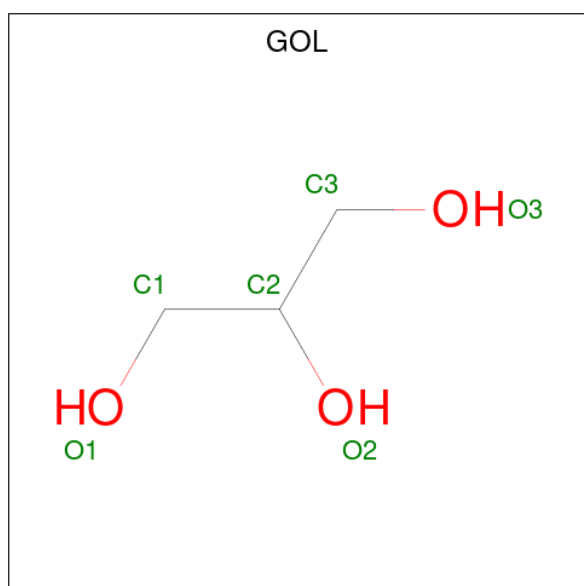
There are 3 unique types of molecules in this entry. The entry contains 6209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycosyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2889	1818	528	529	14			
1	B	376	Total	C	N	O	S	0	3	0
			2865	1803	527	521	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

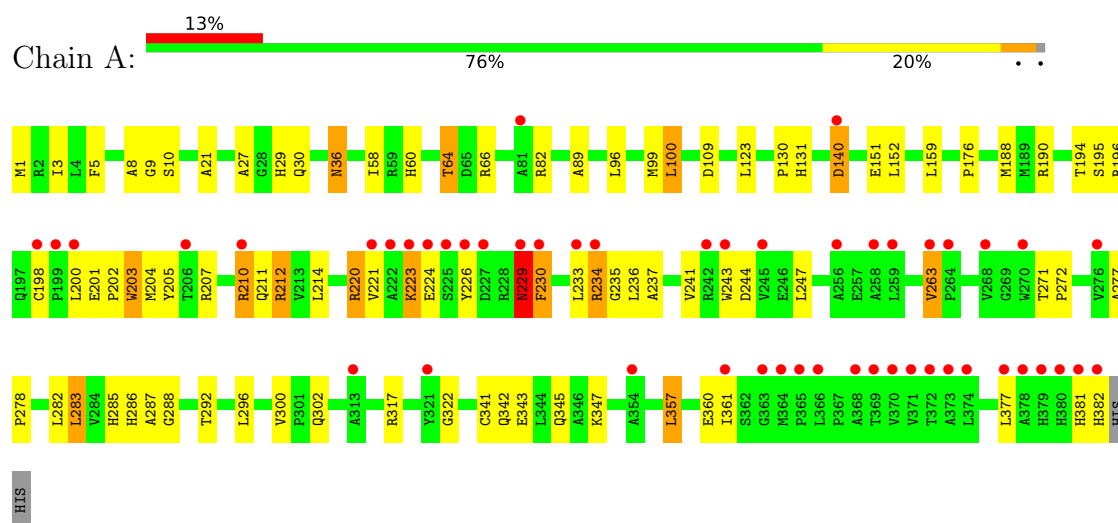
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	202	Total	O	0	0
			202	202		

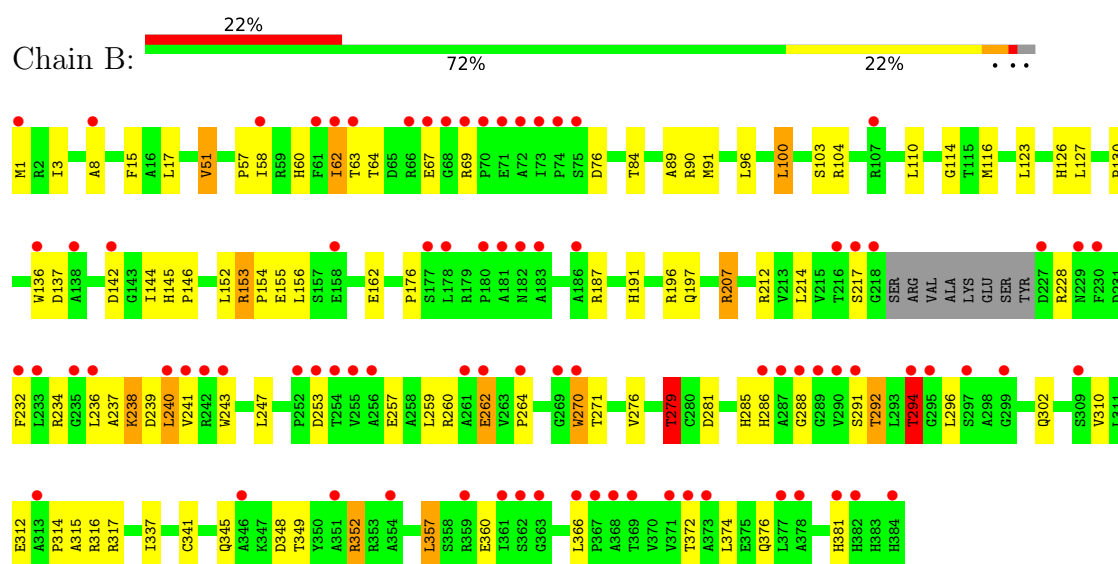
3 Residue-property plots [i](#)

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: Glycosyl transferase



• Molecule 1: Glycosyl transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.87Å 78.90Å 133.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.04 – 1.88 67.99 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (68.04-1.88) 99.7 (67.99-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	6.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.230 0.189 , 0.231	Depositor DCC
R_{free} test set	2868 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: GOL

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	0.86	1/2958 (0.0%)	0.99	4/4046 (0.1%)
1	B	0.84	0/2944	1.00	7/4025 (0.2%)
All	All	0.85	1/5902 (0.0%)	1.00	11/8071 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	TRP	N-CA	5.03	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASN	CA-C-N	7.32	134.88	121.70
1	A	229	ASN	C-N-CA	7.32	134.88	121.70
1	B	207	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	A	210	ARG	N-CA-C	-6.52	100.39	110.10
1	B	279	THR	N-CA-CB	-6.28	101.17	110.53
1	B	76	ASP	CA-C-N	5.44	124.90	119.24
1	B	76	ASP	C-N-CA	5.44	124.90	119.24
1	B	294	THR	N-CA-CB	5.19	117.84	110.16
1	A	198	CYS	O-C-N	5.07	127.15	121.32
1	B	292	THR	N-CA-C	-5.03	106.40	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ALA	N-CA-C	-5.01	105.53	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ARG	Peptide
1	A	229	ASN	Peptide

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	2889	0	2896	69	0
1	B	2865	0	2868	70	1
2	A	30	0	40	8	0
2	B	12	0	16	2	0
3	A	211	0	0	12	0
3	B	202	0	0	17	0
All	All	6209	0	5820	141	1

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 12.

All (141) 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:207:ARG:HG2	3:A:1151:HOH:O	1.60	1.01
1:B:291:SER:O	3:B:1157:HOH:O	1.79	0.99
1:B:84:THR:HG22	1:B:116:MET:HE1	1.48	0.95
1:A:223:LYS:O	1:A:223:LYS:HG2	1.68	0.93
1:B:317:ARG:HD2	3:B:1126:HOH:O	1.68	0.93
1:B:292:THR:HG21	3:B:1206:HOH:O	1.74	0.85
1:B:212:ARG:HH11	1:B:279:THR:CG2	1.89	0.84
1:B:312:GLU:O	1:B:316:ARG:HG3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:CYS:O	1:B:345:GLN:HG3	1.80	0.80
1:B:285:HIS:CE1	1:B:302:GLN:HE21	2.00	0.79
1:A:196:ARG:HG2	3:A:1061:HOH:O	1.85	0.77
1:A:243:TRP:CZ2	1:A:342:GLN:HG3	2.22	0.73
1:A:203:TRP:CZ2	1:A:271:THR:HG21	2.25	0.72
1:A:203:TRP:O	1:A:212:ARG:NH1	2.23	0.71
1:A:203:TRP:CH2	1:A:271:THR:HG21	2.26	0.70
1:B:212:ARG:HH11	1:B:279:THR:HG23	1.57	0.69
1:B:285:HIS:HE1	1:B:302:GLN:HE21	1.40	0.68
1:A:285:HIS:HD1	1:A:287:ALA:H	1.42	0.67
1:A:223:LYS:O	1:A:223:LYS:CG	2.37	0.67
1:A:109:ASP:O	1:A:382:HIS:HE1	1.77	0.67
1:B:285:HIS:HE1	1:B:302:GLN:NE2	1.93	0.67
1:A:100:LEU:HD13	1:A:123:LEU:HD23	1.77	0.66
1:B:239:ASP:O	3:B:1155:HOH:O	2.12	0.66
1:A:188:MET:HG2	3:A:1098:HOH:O	1.95	0.66
1:B:285:HIS:CE1	1:B:302:GLN:NE2	2.63	0.66
1:A:60:HIS:O	1:A:64:THR:HG23	1.96	0.64
1:A:322:GLY:CA	2:A:1003:GOL:H2	2.27	0.64
1:B:91:MET:HG3	3:B:1026:HOH:O	1.97	0.64
1:B:137:ASP:HB3	3:B:1187:HOH:O	1.95	0.64
1:A:322:GLY:HA3	2:A:1003:GOL:H2	1.78	0.64
1:B:212:ARG:HH11	1:B:279:THR:HG21	1.61	0.63
1:B:103:SER:HB3	1:B:127:LEU:HD11	1.79	0.63
1:A:66:ARG:CD	1:A:151:GLU:OE1	2.48	0.62
1:A:131:HIS:HD2	3:A:1093:HOH:O	1.81	0.61
1:B:288:GLY:HA2	2:B:1004:GOL:H11	1.81	0.61
1:A:36:ASN:H	1:A:36:ASN:HD22	1.47	0.61
1:A:229:ASN:O	1:A:286:HIS:CE1	2.55	0.60
1:B:191:HIS:NE2	1:B:294:THR:HG22	2.18	0.59
1:B:116:MET:HE3	1:B:144:ILE:CG2	2.33	0.59
1:A:10:SER:HB2	1:A:224:GLU:HG3	1.85	0.58
2:B:1004:GOL:H11	3:B:1154:HOH:O	2.03	0.58
1:A:1:MET:HE3	1:A:3:ILE:HD11	1.86	0.58
1:B:207:ARG:HD2	3:B:1006:HOH:O	2.03	0.57
1:A:96:LEU:HG	1:A:100:LEU:HD22	1.84	0.57
1:B:187:ARG:HD2	3:B:1013:HOH:O	2.04	0.56
1:B:187:ARG:CD	3:B:1013:HOH:O	2.53	0.56
1:A:29:HIS:CE1	2:A:1007:GOL:H11	2.40	0.56
1:A:292:THR:HA	1:A:302:GLN:HE22	1.71	0.56
1:B:197:GLN:NE2	3:B:1041:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1007:GOL:H32	3:A:1202:HOH:O	2.07	0.55
1:B:207:ARG:HH22	1:B:281:ASP:CG	2.14	0.55
1:B:296:LEU:HD22	1:B:357:LEU:HD23	1.88	0.55
1:B:116:MET:HE3	1:B:144:ILE:HG21	1.89	0.54
1:A:220:ARG:H	1:A:220:ARG:HH21	1.56	0.54
1:A:237:ALA:CB	1:A:263:VAL:HG21	2.38	0.54
1:A:109:ASP:O	1:A:382:HIS:CE1	2.59	0.54
1:A:229:ASN:HA	1:A:230:PHE:HB2	1.89	0.54
1:B:110:LEU:HD21	1:B:374:LEU:HD22	1.90	0.54
1:B:270:TRP:N	1:B:270:TRP:CD1	2.75	0.54
1:A:341:CYS:O	1:A:345:GLN:HB2	2.08	0.53
1:B:63:THR:HG22	1:B:64:THR:N	2.23	0.53
1:A:82:ARG:NH1	3:A:1123:HOH:O	2.42	0.53
1:A:66:ARG:HD2	1:A:151:GLU:OE1	2.09	0.52
1:B:217:SER:OG	1:B:286:HIS:HD2	1.92	0.52
1:B:126:HIS:HE1	3:B:1039:HOH:O	1.93	0.52
1:B:212:ARG:NH1	1:B:279:THR:CG2	2.67	0.52
1:B:63:THR:HG22	1:B:64:THR:H	1.74	0.51
1:A:130:PRO:HG3	1:A:381:HIS:CG	2.45	0.51
1:A:277:ALA:HB3	1:A:278:PRO:HD3	1.93	0.51
1:B:348[A]:ASP:OD2	1:B:352:ARG:HD3	2.11	0.51
1:B:212:ARG:NH1	1:B:279:THR:HG21	2.26	0.51
1:B:276:VAL:O	1:B:279:THR:HB	2.11	0.50
1:A:140:ASP:HB3	3:A:1080:HOH:O	2.09	0.50
1:A:9:GLY:HA3	1:A:58:ILE:CG2	2.42	0.50
1:A:201:GLU:HB2	1:A:204:MET:HE3	1.93	0.50
1:A:60:HIS:HD2	3:A:1130:HOH:O	1.94	0.50
1:B:1:MET:HE2	1:B:3:ILE:HG12	1.93	0.49
1:A:9:GLY:HA3	1:A:58:ILE:HG23	1.95	0.49
1:A:296:LEU:HD22	1:A:357:LEU:HD23	1.94	0.49
1:A:229:ASN:C	1:A:229:ASN:HD22	2.21	0.48
1:A:202:PRO:HA	1:A:205:TYR:CZ	2.48	0.48
1:A:286:HIS:HE1	3:A:1124:HOH:O	1.97	0.47
1:B:372:THR:HG22	1:B:376:GLN:HE21	1.79	0.47
1:A:36:ASN:HD22	1:A:36:ASN:N	2.11	0.47
1:A:223:LYS:HG3	3:A:1041:HOH:O	2.15	0.47
2:A:1006:GOL:C3	3:A:1142:HOH:O	2.62	0.47
1:A:220:ARG:H	1:A:220:ARG:NH2	2.13	0.47
1:A:195:SER:OG	1:A:272:PRO:HB3	2.14	0.46
1:B:100:LEU:O	1:B:104:ARG:HG3	2.15	0.46
1:A:60:HIS:CD2	3:A:1130:HOH:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HB2	1:B:51:VAL:HG23	1.97	0.46
1:B:96:LEU:O	1:B:100:LEU:HB2	2.16	0.46
1:B:243:TRP:CD1	3:B:1155:HOH:O	2.67	0.46
1:B:257:GLU:HG2	1:B:260:ARG:HH21	1.80	0.46
1:A:237:ALA:O	1:A:241:VAL:HG23	2.16	0.45
1:B:100:LEU:HD13	1:B:123:LEU:HD23	1.98	0.45
1:B:89:ALA:HB1	1:B:152:LEU:HG	1.98	0.45
1:B:214:LEU:C	1:B:214:LEU:HD23	2.42	0.45
1:B:153:ARG:HB3	1:B:154:PRO:HD3	1.99	0.45
1:B:1:MET:HE1	1:B:110:LEU:HB3	2.00	0.44
1:B:314:PRO:HB2	3:B:1079:HOH:O	2.17	0.44
1:B:212:ARG:NH1	1:B:279:THR:HG23	2.28	0.44
1:B:236:LEU:HD13	1:B:337:ILE:HG21	2.00	0.44
1:A:243:TRP:CH2	1:A:342:GLN:HG3	2.52	0.43
1:B:243:TRP:HB2	3:B:1155:HOH:O	2.17	0.43
1:B:262:GLU:O	1:B:264:PRO:HD3	2.18	0.43
1:A:322:GLY:HA2	2:A:1003:GOL:H2	1.99	0.43
1:A:30:GLN:NE2	2:A:1006:GOL:O3	2.51	0.43
1:A:243:TRP:HZ2	1:A:342:GLN:HG3	1.81	0.43
1:B:232:PHE:CZ	1:B:236:LEU:HD22	2.54	0.43
1:A:27:ALA:O	2:A:1007:GOL:H31	2.18	0.43
1:B:292:THR:HG23	3:B:1095:HOH:O	2.19	0.43
1:A:263:VAL:HG22	1:A:263:VAL:O	2.19	0.42
1:B:62:ILE:HA	1:B:90:ARG:HH21	1.84	0.42
1:A:190:ARG:HG3	1:A:361:ILE:O	2.19	0.42
1:B:234:ARG:NH1	1:B:238:LYS:HE2	2.34	0.42
1:A:343:GLU:HG3	1:A:347:LYS:HG3	2.02	0.42
1:A:1:MET:HE3	1:A:3:ILE:CD1	2.49	0.42
1:A:226:TYR:CE1	1:A:288:GLY:HA3	2.55	0.42
1:A:229:ASN:C	1:A:229:ASN:ND2	2.78	0.42
1:B:15:PHE:HZ	1:B:196[A]:ARG:HG3	1.84	0.42
1:B:142:ASP:OD2	1:B:142:ASP:C	2.62	0.42
1:B:276:VAL:O	1:B:279:THR:HG22	2.20	0.42
1:A:140:ASP:OD1	1:A:317:ARG:NH1	2.49	0.42
1:A:5:PHE:CZ	1:A:21:ALA:HA	2.55	0.42
1:A:234:ARG:HG2	1:A:235:GLY:N	2.35	0.42
1:A:285:HIS:NE2	1:A:302:GLN:NE2	2.68	0.42
1:B:57:PRO:HD2	1:B:60:HIS:ND1	2.35	0.42
1:B:237:ALA:HA	1:B:247:LEU:CD2	2.50	0.41
1:B:234:ARG:HE	1:B:262:GLU:HG2	1.84	0.41
1:B:240:LEU:HD23	1:B:247:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA3	1:B:136:TRP:CE3	2.55	0.41
1:B:176:PRO:HD2	1:B:360:GLU:OE2	2.21	0.41
1:A:89:ALA:HB1	1:A:152:LEU:HG	2.02	0.41
1:B:196[A]:ARG:NH1	3:B:1104:HOH:O	2.54	0.41
1:B:130:PRO:HG3	1:B:381[B]:HIS:CG	2.55	0.41
1:A:99:MET:HB3	1:A:123:LEU:HD11	2.04	0.40
1:A:226:TYR:CZ	1:A:288:GLY:HA3	2.57	0.40
1:A:283:LEU:HD13	1:A:300:VAL:HG11	2.04	0.40
1:B:145:HIS:N	1:B:146:PRO:CD	2.84	0.40
1:A:176:PRO:HD2	1:A:360:GLU:OE1	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLU:OE2	1:B:349:THR:OG1[3_656]	2.06	0.14

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	380/384 (99%)	369 (97%)	6 (2%)	5 (1%)	9	2
1	B	375/384 (98%)	364 (97%)	10 (3%)	1 (0%)	36	26
All	All	755/768 (98%)	733 (97%)	16 (2%)	6 (1%)	16	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	244	ASP
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	230	PHE
1	B	8	ALA
1	A	8	ALA

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	300/302 (99%)	279 (93%)	21 (7%)	14	3
1	B	298/302 (99%)	273 (92%)	25 (8%)	10	2
All	All	598/604 (99%)	552 (92%)	46 (8%)	12	2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	64	THR
1	A	100	LEU
1	A	140	ASP
1	A	159	LEU
1	A	194	THR
1	A	212	ARG
1	A	214	LEU
1	A	220	ARG
1	A	221	VAL
1	A	223	LYS
1	A	229	ASN
1	A	233	LEU
1	A	234	ARG
1	A	236	LEU
1	A	247	LEU
1	A	263	VAL
1	A	282	LEU
1	A	283	LEU
1	A	357	LEU

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Mol	Chain	Res	Type
1	A	377	LEU
1	B	17	LEU
1	B	51	VAL
1	B	58	ILE
1	B	62	ILE
1	B	67	GLU
1	B	69	ARG
1	B	100	LEU
1	B	153	ARG
1	B	156	LEU
1	B	162	GLU
1	B	228	ARG
1	B	238	LYS
1	B	240	LEU
1	B	241	VAL
1	B	253	ASP
1	B	259	LEU
1	B	262	GLU
1	B	270	TRP
1	B	271	THR
1	B	279	THR
1	B	294	THR
1	B	310	VAL
1	B	352	ARG
1	B	357	LEU
1	B	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	36	ASN
1	A	131	HIS
1	A	134	GLN
1	A	229	ASN
1	A	286	HIS
1	A	302	GLN
1	A	381	HIS
1	A	382	HIS
1	B	37	GLN
1	B	126	HIS
1	B	131	HIS

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Mol	Chain	Res	Type
1	B	197	GLN
1	B	229	ASN
1	B	285	HIS
1	B	286	HIS
1	B	302	GLN
1	B	376	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands 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	GOL	A	1003	-	5,5,5	0.52	0	5,5,5	0.90	0
2	GOL	A	1006	-	5,5,5	0.24	0	5,5,5	1.29	1 (20%)
2	GOL	A	1007	-	5,5,5	0.33	0	5,5,5	0.64	0
2	GOL	B	1001	-	5,5,5	0.48	0	5,5,5	0.27	0
2	GOL	A	1002	-	5,5,5	0.49	0	5,5,5	0.95	0
2	GOL	B	1004	-	5,5,5	0.46	0	5,5,5	0.41	0
2	GOL	A	1005	-	5,5,5	0.52	0	5,5,5	0.95	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	GOL	A	1003	-	-	2/4/4/4	-
2	GOL	A	1006	-	-	2/4/4/4	-
2	GOL	A	1007	-	-	2/4/4/4	-
2	GOL	B	1001	-	-	0/4/4/4	-
2	GOL	A	1002	-	-	3/4/4/4	-
2	GOL	B	1004	-	-	2/4/4/4	-
2	GOL	A	1005	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1006	GOL	C3-C2-C1	-2.12	104.00	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	GOL	C1-C2-C3-O3
2	A	1006	GOL	C1-C2-C3-O3
2	A	1006	GOL	O2-C2-C3-O3
2	A	1007	GOL	O1-C1-C2-C3
2	B	1004	GOL	C1-C2-C3-O3
2	A	1002	GOL	O1-C1-C2-C3
2	A	1002	GOL	C1-C2-C3-O3
2	A	1002	GOL	O2-C2-C3-O3
2	B	1004	GOL	O2-C2-C3-O3
2	A	1007	GOL	O1-C1-C2-O2
2	A	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	GOL	3	0
2	A	1006	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1007	GOL	3	0
2	B	1004	GOL	2	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

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	382/384 (99%)	0.86	50 (13%) 7 8	22, 28, 39, 47	0
1	B	376/384 (97%)	1.19	83 (22%) 2 2	15, 28, 44, 51	3 (0%)
All	All	758/768 (98%)	1.03	133 (17%) 4 4	15, 28, 42, 51	3 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	GLY	5.7
1	B	270	TRP	5.6
1	B	287	ALA	5.5
1	B	289	GLY	5.4
1	A	382	HIS	4.9
1	B	73	ILE	4.4
1	B	74	PRO	4.2
1	A	363	GLY	4.2
1	A	270	TRP	4.1
1	B	241	VAL	4.0
1	B	181	ALA	4.0
1	A	243	TRP	4.0
1	B	136	TRP	4.0
1	A	377	LEU	4.0
1	B	72	ALA	4.0
1	B	230	PHE	3.9
1	B	261	ALA	3.6
1	B	158	GLU	3.6
1	A	224	GLU	3.5
1	B	243	TRP	3.5
1	B	290	VAL	3.4
1	B	369	THR	3.4
1	A	378	ALA	3.3
1	A	373	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	142	ASP	3.3
1	B	291	SER	3.3
1	B	70	PRO	3.2
1	B	217	SER	3.2
1	B	183	ALA	3.2
1	B	366	LEU	3.2
1	B	232	PHE	3.2
1	A	361	ILE	3.1
1	A	372	THR	3.1
1	B	63	THR	3.1
1	A	369	THR	3.1
1	B	252	PRO	3.1
1	B	368	ALA	3.1
1	B	269	GLY	3.0
1	B	371	VAL	3.0
1	A	222	ALA	3.0
1	B	372	THR	2.9
1	B	288	GLY	2.9
1	A	245	VAL	2.9
1	B	182	ASN	2.9
1	A	313	ALA	2.9
1	B	138	ALA	2.9
1	B	233	LEU	2.9
1	A	229	ASN	2.8
1	A	223	LYS	2.8
1	B	229	ASN	2.8
1	B	254	THR	2.8
1	A	221	VAL	2.8
1	B	107	ARG	2.8
1	B	71	GLU	2.8
1	B	361	ILE	2.8
1	A	258	ALA	2.7
1	A	199	PRO	2.7
1	A	365	PRO	2.7
1	B	177	SER	2.7
1	B	313	ALA	2.6
1	B	382	HIS	2.6
1	B	235	GLY	2.6
1	A	371	VAL	2.6
1	B	309	SER	2.6
1	B	286	HIS	2.5
1	B	8	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	263	VAL	2.5
1	A	380	HIS	2.5
1	B	363	GLY	2.5
1	A	381	HIS	2.5
1	B	180	PRO	2.5
1	B	227	ASP	2.5
1	B	354	ALA	2.5
1	A	242	ARG	2.4
1	B	299	GLY	2.4
1	A	379	HIS	2.4
1	B	262	GLU	2.4
1	A	226	TYR	2.4
1	A	259	LEU	2.4
1	A	230	PHE	2.4
1	B	62	ILE	2.4
1	A	366	LEU	2.4
1	A	368	ALA	2.4
1	A	370	VAL	2.4
1	A	354	ALA	2.3
1	B	256	ALA	2.3
1	A	276	VAL	2.3
1	B	236	LEU	2.3
1	B	367	PRO	2.3
1	A	210	ARG	2.3
1	B	377	LEU	2.3
1	A	227	ASP	2.3
1	B	240	LEU	2.3
1	B	294	THR	2.3
1	A	234	ARG	2.2
1	B	359	ARG	2.2
1	B	58	ILE	2.2
1	A	256	ALA	2.2
1	B	346	ALA	2.2
1	B	378	ALA	2.2
1	B	381[A]	HIS	2.2
1	B	384	HIS	2.2
1	B	68	GLY	2.2
1	B	253	ASP	2.2
1	B	297	SER	2.2
1	B	1	MET	2.2
1	B	255	VAL	2.2
1	B	216	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	2.2
1	B	66	ARG	2.2
1	A	268	VAL	2.1
1	B	362	SER	2.1
1	A	233	LEU	2.1
1	A	374	LEU	2.1
1	A	206	THR	2.1
1	B	295	GLY	2.1
1	B	67	GLU	2.1
1	A	81	ALA	2.1
1	B	351	ALA	2.1
1	B	373	ALA	2.1
1	B	69	ARG	2.1
1	B	75	SER	2.1
1	B	264	PRO	2.1
1	A	198	CYS	2.1
1	B	178	LEU	2.1
1	B	186	ALA	2.1
1	A	225	SER	2.0
1	A	321	TYR	2.0
1	A	364	MET	2.0
1	A	140	ASP	2.0
1	B	61	PHE	2.0
1	A	264	PRO	2.0
1	B	242	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

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, 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	1003	6/6	0.74	0.15	37,43,44,47	0
2	GOL	B	1004	6/6	0.79	0.17	39,41,41,42	0
2	GOL	A	1002	6/6	0.81	0.17	37,39,41,41	0
2	GOL	A	1006	6/6	0.82	0.14	36,40,40,46	0
2	GOL	A	1007	6/6	0.85	0.14	51,52,52,52	0
2	GOL	A	1005	6/6	0.93	0.15	29,30,33,33	0
2	GOL	B	1001	6/6	0.95	0.13	19,21,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.