



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:10 PM BST

PDB ID : 6OYC
Title : Glycosylation Associate Protein (Gap123) complex from *Streptococcus agalactiae*
Authors : zhang, H.; Wu, H.
Deposited on : 2019-05-14
Resolution : 2.35 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

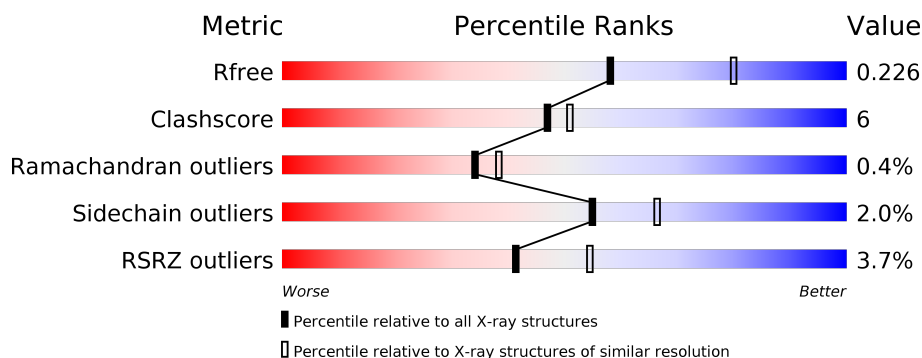
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	514	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 11%, green 84%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 86% 11% • • </div> </div>
2	B	519	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 15%, green 84%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 84% 15% • </div> </div>
3	C	330	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 16%, green 77%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 77% 16% • 6% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11323 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 Glycosylation Associate Protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4150	2671	686	784	9			

- Molecule 2 is a protein called Glycosylation Associate Protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	517	Total	C	N	O	S	0	0	0
			4163	2677	685	789	12			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q8DYM5
B	2	SER	-	expression tag	UNP Q8DYM5
B	3	LYS	-	expression tag	UNP Q8DYM5
B	4	ILE	-	expression tag	UNP Q8DYM5
B	5	LYS	-	expression tag	UNP Q8DYM5
B	6	LEU	-	expression tag	UNP Q8DYM5
B	7	THR	-	expression tag	UNP Q8DYM5
B	8	ILE	-	expression tag	UNP Q8DYM5
B	9	LEU	-	expression tag	UNP Q8DYM5
B	10	GLN	-	expression tag	UNP Q8DYM5
B	11	VAL	-	expression tag	UNP Q8DYM5
B	12	GLY	-	expression tag	UNP Q8DYM5
B	13	GLU	-	expression tag	UNP Q8DYM5
B	14	GLU	-	expression tag	UNP Q8DYM5
B	15	ASN	-	expression tag	UNP Q8DYM5
B	16	TRP	-	expression tag	UNP Q8DYM5
B	17	ALA	-	expression tag	UNP Q8DYM5
B	18	THR	-	expression tag	UNP Q8DYM5
B	19	LYS	-	expression tag	UNP Q8DYM5
B	20	GLU	-	expression tag	UNP Q8DYM5

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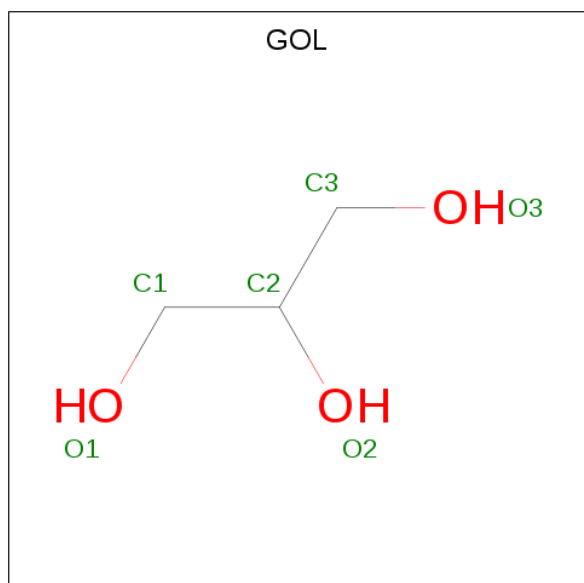
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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASN	-	expression tag	UNP Q8DYM5
B	22	ILE	-	expression tag	UNP Q8DYM5
B	23	PRO	-	expression tag	UNP Q8DYM5
B	24	ASN	-	expression tag	UNP Q8DYM5
B	25	ASN	-	expression tag	UNP Q8DYM5

- Molecule 3 is a protein called Glycosylation Associate Protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	310	Total	C	N	O	S	0	0	0
			2514	1632	402	476	4			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



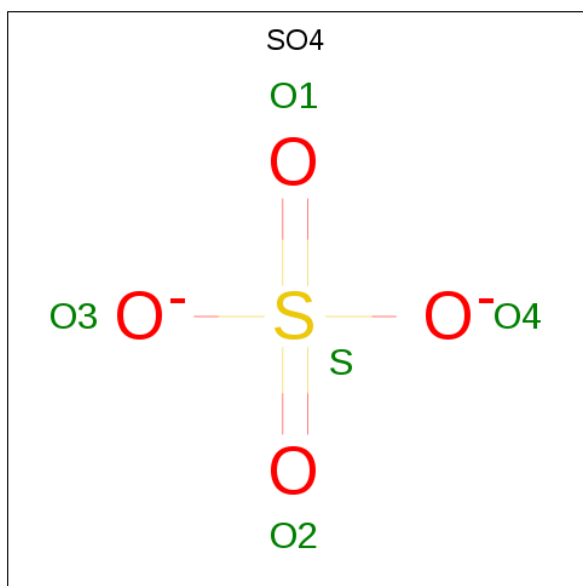
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

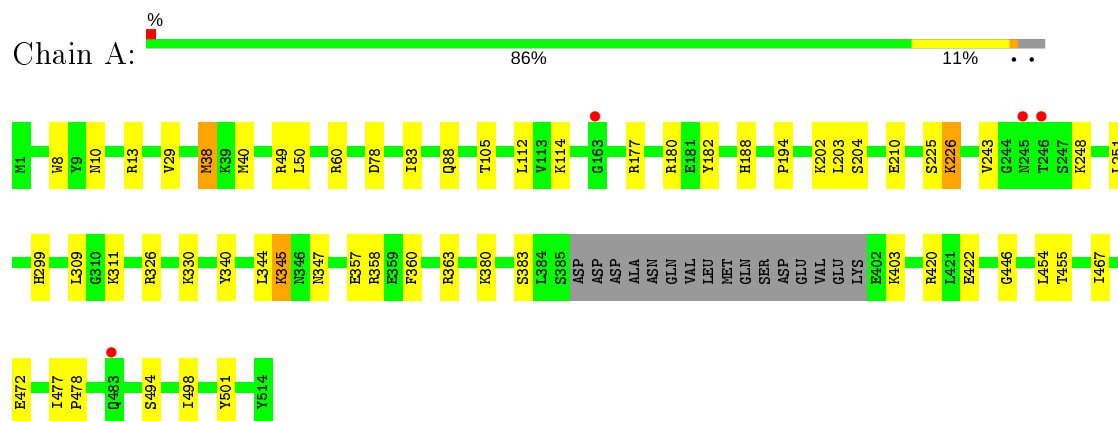
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	166	Total 166	O 166	0	0
6	B	172	Total 172	O 172	0	0
6	C	65	Total 65	O 65	0	0

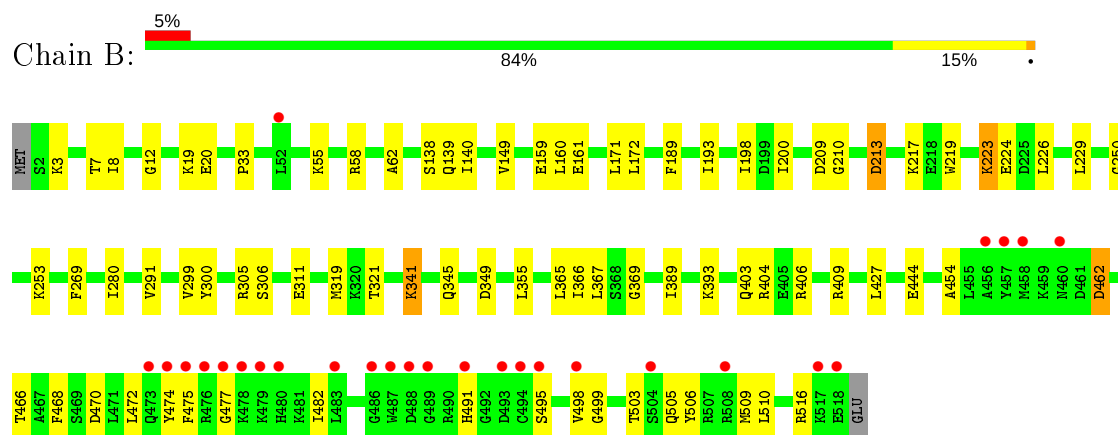
3 Residue-property plots [i](#)

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.

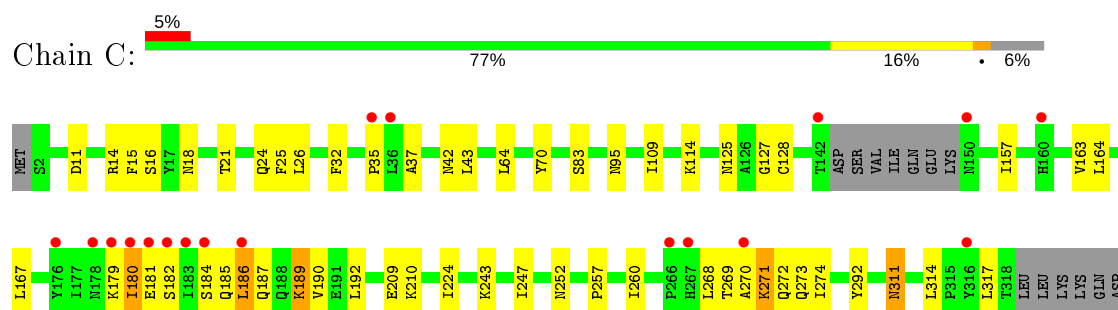
• Molecule 1: Glycosylation Associate Protein 1



• Molecule 2: Glycosylation Associate Protein 2



• Molecule 3: Glycosylation Associate Protein 3



ASP
ASN
TYR
ASP
SER
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.01Å 168.32Å 100.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.35 49.27 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.27-2.35) 99.6 (49.27-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_3051: ???)	Depositor
R, R_{free}	0.181 , 0.227 0.181 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11323	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.43	0/4246	0.58	0/5744
2	B	0.46	0/4263	0.56	1/5750 (0.0%)
3	C	0.42	0/2573	0.61	1/3492 (0.0%)
All	All	0.44	0/11082	0.58	2/14986 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	186	LEU	CA-CB-CG	5.52	128.00	115.30
2	B	55	LYS	C-N-CA	-5.11	108.94	121.70

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	4150	0	4067	39	0
2	B	4163	0	4046	53	0
3	C	2514	0	2507	47	0
4	A	36	0	48	10	0
4	B	24	0	32	3	0
4	C	18	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	166	0	0	4	0
6	B	172	0	0	2	0
6	C	65	0	0	0	0
All	All	11323	0	10724	135	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 6.

All (135) 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)
3:C:157:ILE:HD11	3:C:164:LEU:HD22	1.67	0.77
2:B:366:ILE:HD13	2:B:509:MET:HE1	1.66	0.75
3:C:184:SER:HB2	3:C:190:VAL:HG12	1.69	0.74
3:C:269:THR:HG23	3:C:272:GLN:H	1.53	0.73
3:C:186:LEU:HD11	3:C:314:LEU:HB3	1.70	0.73
3:C:24:GLN:HG2	3:C:26:LEU:HG	1.73	0.70
3:C:269:THR:HG21	3:C:271:LYS:HG2	1.75	0.69
2:B:366:ILE:HD11	2:B:509:MET:HE3	1.73	0.69
1:A:38:MET:HE1	1:A:50:LEU:HD13	1.75	0.68
2:B:409:ARG:NH2	6:B:702:HOH:O	2.27	0.67
1:A:311:LYS:NZ	1:A:422:GLU:OE2	2.26	0.67
3:C:179:LYS:O	3:C:180:ILE:HG13	1.95	0.67
1:A:248:LYS:NZ	6:A:701:HOH:O	2.27	0.67
2:B:149:VAL:HG22	2:B:161:GLU:HB3	1.78	0.64
3:C:179:LYS:O	3:C:181:GLU:N	2.20	0.64
3:C:184:SER:CB	3:C:190:VAL:HG12	2.28	0.64
3:C:268:LEU:HD23	3:C:273:GLN:HG3	1.78	0.63
3:C:43:LEU:HD11	3:C:125:ASN:HB2	1.79	0.63
2:B:475:PHE:CD1	2:B:482:ILE:HD11	2.34	0.62
1:A:420:ARG:HG3	6:A:703:HOH:O	1.98	0.62
1:A:299:HIS:H	4:A:605:GOL:H11	1.65	0.62
2:B:366:ILE:CD1	2:B:509:MET:CE	2.77	0.62
2:B:462:ASP:N	2:B:462:ASP:OD2	2.32	0.61
3:C:11:ASP:HB3	3:C:25:PHE:CZ	2.36	0.61
1:A:340:TYR:CE2	1:A:344:LEU:HD11	2.37	0.60
3:C:269:THR:CG2	3:C:271:LYS:HG2	2.32	0.60
3:C:269:THR:HG22	3:C:272:GLN:OE1	2.02	0.60
3:C:18:ASN:OD1	3:C:21:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:ILE:CD1	2:B:509:MET:HE1	2.33	0.59
2:B:193:ILE:HD11	2:B:280:ILE:HB	1.86	0.58
3:C:270:ALA:O	3:C:274:ILE:HD12	2.04	0.57
2:B:366:ILE:HD13	2:B:509:MET:CE	2.34	0.57
2:B:495:SER:HA	2:B:498:VAL:HG12	1.86	0.57
1:A:29:VAL:HA	4:A:606:GOL:H2	1.86	0.57
2:B:159:GLU:HG3	2:B:253:LYS:HG2	1.87	0.56
1:A:326:ARG:HH22	4:A:604:GOL:H32	1.71	0.56
3:C:163:VAL:O	3:C:189:LYS:NZ	2.25	0.56
1:A:49:ARG:HD3	4:A:602:GOL:H11	1.88	0.55
2:B:366:ILE:CD1	2:B:509:MET:HE3	2.38	0.54
3:C:184:SER:O	3:C:186:LEU:N	2.39	0.54
3:C:269:THR:OG1	3:C:270:ALA:N	2.40	0.54
3:C:37:ALA:HB1	3:C:127:GLY:O	2.08	0.54
3:C:179:LYS:HE2	3:C:181:GLU:OE1	2.08	0.53
1:A:114:LYS:HD2	4:A:601:GOL:H12	1.90	0.53
1:A:8:TRP:HA	4:A:606:GOL:H32	1.89	0.53
1:A:78:ASP:HA	1:A:83:ILE:HD12	1.90	0.53
2:B:198:ILE:HD11	2:B:250:GLY:C	2.29	0.53
1:A:446:GLY:HA2	1:A:494:SER:OG	2.09	0.53
2:B:495:SER:O	2:B:498:VAL:HG12	2.08	0.53
2:B:499:GLY:O	2:B:503:THR:HG22	2.09	0.53
2:B:140:ILE:HG23	2:B:172:LEU:HD13	1.90	0.53
2:B:355:LEU:HD11	2:B:365:LEU:HD22	1.91	0.52
1:A:358:ARG:HH22	4:A:603:GOL:H12	1.75	0.52
2:B:475:PHE:O	2:B:477:GLY:N	2.39	0.52
2:B:8:ILE:HD12	2:B:62:ALA:HB3	1.92	0.51
3:C:11:ASP:N	3:C:11:ASP:OD1	2.42	0.51
2:B:19:LYS:HG2	2:B:20:GLU:HG2	1.93	0.51
1:A:360:PHE:HD2	2:B:210:GLY:O	1.94	0.50
1:A:243:VAL:HG13	1:A:251:LEU:HD21	1.92	0.50
3:C:257:PRO:HD2	3:C:260:ILE:HD12	1.94	0.50
3:C:95:ASN:OD1	4:C:402:GOL:H11	2.11	0.50
1:A:49:ARG:HH11	4:A:602:GOL:H12	1.77	0.50
2:B:19:LYS:HE3	2:B:20:GLU:OE2	2.12	0.49
2:B:200:ILE:HG13	2:B:226:LEU:HD12	1.93	0.49
2:B:444:GLU:HG2	2:B:474:TYR:HE2	1.77	0.49
1:A:112:LEU:HD11	2:B:213:ASP:HB2	1.95	0.49
2:B:403:GLN:O	2:B:406:ARG:HD3	2.12	0.49
2:B:366:ILE:HD11	2:B:509:MET:CE	2.37	0.49
1:A:202:LYS:NZ	1:A:210:GLU:OE2	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:VAL:HB	2:B:367:LEU:HD23	1.95	0.49
1:A:357:GLU:O	1:A:363:ARG:HD3	2.13	0.48
2:B:189:PHE:HB2	2:B:229:LEU:HD12	1.95	0.48
2:B:345:GLN:NE2	2:B:349:ASP:OD1	2.43	0.48
2:B:306:SER:H	4:B:602:GOL:H12	1.78	0.48
3:C:224:ILE:HB	3:C:247:ILE:HG22	1.95	0.47
2:B:475:PHE:CE1	2:B:482:ILE:HD11	2.48	0.47
3:C:186:LEU:HD23	3:C:187:GLN:N	2.28	0.47
3:C:167:LEU:HB2	3:C:190:VAL:HG21	1.95	0.47
3:C:268:LEU:HD23	3:C:273:GLN:CG	2.45	0.47
2:B:341:LYS:CE	2:B:341:LYS:H	2.28	0.47
2:B:427:LEU:HB2	3:C:35:PRO:HD2	1.97	0.47
2:B:454:ALA:HB1	2:B:505:GLN:HG2	1.96	0.47
1:A:420:ARG:NH1	6:A:703:HOH:O	2.34	0.47
1:A:105:THR:HB	1:A:112:LEU:HB2	1.96	0.47
1:A:498:ILE:O	1:A:501:TYR:HB3	2.15	0.47
2:B:367:LEU:O	2:B:389:ILE:HA	2.15	0.47
3:C:14:ARG:HD3	3:C:15:PHE:CE2	2.50	0.46
2:B:306:SER:H	4:B:602:GOL:H32	1.80	0.46
1:A:345:LYS:HE2	1:A:345:LYS:HB3	1.74	0.46
1:A:49:ARG:NH2	6:A:705:HOH:O	2.39	0.46
2:B:160:LEU:HD13	2:B:171:LEU:HD21	1.97	0.45
3:C:269:THR:OG1	3:C:271:LYS:HE3	2.15	0.45
1:A:467:ILE:HB	1:A:472:GLU:HB3	1.98	0.45
2:B:305:ARG:HH11	2:B:311:GLU:HG3	1.80	0.45
1:A:177:ARG:NH1	1:A:180:ARG:HH21	2.15	0.45
1:A:10:ASN:HB3	1:A:13:ARG:O	2.16	0.45
2:B:139:GLN:NE2	6:B:708:HOH:O	2.49	0.45
2:B:393:LYS:HB3	2:B:491:HIS:CE1	2.53	0.44
3:C:83:SER:OG	3:C:128:CYS:HB2	2.16	0.44
1:A:226:LYS:HD2	1:A:226:LYS:H	1.83	0.44
2:B:319:MET:HB2	2:B:321:THR:HG22	1.99	0.44
3:C:179:LYS:O	3:C:181:GLU:HG2	2.17	0.44
3:C:179:LYS:C	3:C:181:GLU:H	2.16	0.43
3:C:269:THR:CG2	3:C:272:GLN:H	2.27	0.43
1:A:49:ARG:HH11	4:A:602:GOL:C1	2.31	0.43
2:B:306:SER:N	4:B:602:GOL:H12	2.34	0.43
1:A:454:LEU:HD22	1:A:455:THR:H	1.83	0.43
2:B:138:SER:HB3	3:C:16:SER:HB2	2.01	0.43
3:C:314:LEU:O	3:C:317:LEU:HB2	2.17	0.43
3:C:252:ASN:HA	3:C:292:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TYR:O	1:A:188:HIS:HA	2.19	0.42
2:B:468:PHE:CZ	2:B:472:LEU:HD11	2.55	0.42
2:B:12:GLY:O	2:B:33:PRO:HD3	2.20	0.42
2:B:7:THR:O	2:B:8:ILE:HD13	2.20	0.42
2:B:466:THR:OG1	2:B:470:ASP:OD2	2.38	0.41
1:A:38:MET:HE2	1:A:38:MET:HB2	1.93	0.41
2:B:217:LYS:HG2	2:B:219:TRP:CZ2	2.55	0.41
3:C:182:SER:O	3:C:185:GLN:HG2	2.20	0.41
1:A:40:MET:HE2	1:A:501:TYR:CD2	2.55	0.41
3:C:70:TYR:O	3:C:109:ILE:HA	2.19	0.41
3:C:180:ILE:HD11	3:C:311:ASN:O	2.21	0.41
1:A:49:ARG:HD3	4:A:602:GOL:H32	2.02	0.41
3:C:32:PHE:CD1	3:C:32:PHE:C	2.93	0.41
1:A:380:LYS:O	1:A:383:SER:OG	2.37	0.41
1:A:477:ILE:HB	1:A:478:PRO:HD3	2.02	0.41
3:C:167:LEU:HD23	3:C:192:LEU:HD22	2.03	0.41
3:C:64:LEU:HD22	3:C:70:TYR:CE1	2.56	0.41
2:B:223:LYS:HB2	2:B:224:GLU:H	1.64	0.40
3:C:125:ASN:OD1	3:C:128:CYS:HB3	2.21	0.40
3:C:186:LEU:CD2	3:C:187:GLN:H	2.34	0.40
1:A:40:MET:HE2	1:A:501:TYR:HD2	1.87	0.40
2:B:510:LEU:HB3	2:B:516:ARG:HB2	2.03	0.40
3:C:209:GLU:OE1	3:C:243:LYS:HE3	2.21	0.40
1:A:194:PRO:HA	1:A:203:LEU:HD11	2.02	0.40
2:B:300:TYR:CE1	2:B:369:GLY:HA2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/514 (96%)	483 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	515/519 (99%)	493 (96%)	18 (4%)	4 (1%)	19	20
3	C	306/330 (93%)	285 (93%)	20 (6%)	1 (0%)	41	47
All	All	1315/1363 (96%)	1261 (96%)	49 (4%)	5 (0%)	34	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	LYS
3	C	180	ILE
2	B	291	VAL
2	B	213	ASP
2	B	269	PHE

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	460/475 (97%)	449 (98%)	11 (2%)	49	59
2	B	447/450 (99%)	440 (98%)	7 (2%)	62	75
3	C	287/307 (94%)	281 (98%)	6 (2%)	53	65
All	All	1194/1232 (97%)	1170 (98%)	24 (2%)	55	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MET
1	A	60	ARG
1	A	88	GLN
1	A	204	SER
1	A	225	SER
1	A	226	LYS
1	A	309	LEU
1	A	330	LYS
1	A	345	LYS

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	403	LYS
2	B	3	LYS
2	B	58	ARG
2	B	209	ASP
2	B	341	LYS
2	B	404	ARG
2	B	462	ASP
2	B	506	TYR
3	C	42	ASN
3	C	114	LYS
3	C	189	LYS
3	C	210	LYS
3	C	271	LYS
3	C	311	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
3	C	187	GLN
3	C	311	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
4	GOL	C	403	-	5,5,5	0.83	0	5,5,5	0.97	0
4	GOL	A	603	-	5,5,5	0.89	0	5,5,5	0.90	0
4	GOL	B	603	-	5,5,5	0.91	0	5,5,5	1.11	0
4	GOL	B	604	-	5,5,5	0.95	0	5,5,5	1.08	0
4	GOL	A	606	-	5,5,5	1.08	0	5,5,5	1.03	0
4	GOL	C	401	-	5,5,5	0.77	0	5,5,5	1.04	0
4	GOL	A	605	-	5,5,5	0.90	0	5,5,5	1.03	0
4	GOL	A	602	-	5,5,5	0.80	0	5,5,5	1.02	0
5	SO4	A	608	-	4,4,4	0.17	0	6,6,6	0.25	0
4	GOL	A	601	-	5,5,5	1.04	1 (20%)	5,5,5	1.08	0
5	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.14	0
4	GOL	B	601	-	5,5,5	0.76	0	5,5,5	0.93	0
4	GOL	A	604	-	5,5,5	1.03	0	5,5,5	1.17	0
4	GOL	B	602	-	5,5,5	0.99	0	5,5,5	1.05	0
4	GOL	C	402	-	5,5,5	1.15	0	5,5,5	0.70	0
5	SO4	B	605	-	4,4,4	0.08	0	6,6,6	0.20	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	GOL	C	403	-	-	0/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	B	604	-	-	2/4/4/4	-
4	GOL	A	606	-	-	4/4/4/4	-
4	GOL	C	401	-	-	0/4/4/4	-
4	GOL	A	605	-	-	2/4/4/4	-
4	GOL	A	602	-	-	2/4/4/4	-
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	B	601	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	B	602	-	-	4/4/4/4	-
4	GOL	C	402	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	GOL	C3-C2	2.09	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	GOL	C1-C2-C3-O3
4	B	603	GOL	C1-C2-C3-O3
4	A	606	GOL	O1-C1-C2-C3
4	A	606	GOL	C1-C2-C3-O3
4	A	605	GOL	O1-C1-C2-C3
4	A	602	GOL	O1-C1-C2-O2
4	A	602	GOL	O1-C1-C2-C3
4	A	604	GOL	O1-C1-C2-C3
4	B	602	GOL	O1-C1-C2-C3
4	C	402	GOL	O1-C1-C2-O2
4	B	602	GOL	C1-C2-C3-O3
4	C	402	GOL	O1-C1-C2-C3
4	A	603	GOL	O2-C2-C3-O3
4	A	605	GOL	O1-C1-C2-O2
4	B	602	GOL	O1-C1-C2-O2
4	B	602	GOL	O2-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
4	A	606	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	A	606	GOL	O1-C1-C2-O2
4	B	604	GOL	C1-C2-C3-O3
4	C	402	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	GOL	1	0
4	A	606	GOL	2	0
4	A	605	GOL	1	0
4	A	602	GOL	4	0
4	A	601	GOL	1	0
4	A	604	GOL	1	0
4	B	602	GOL	3	0
4	C	402	GOL	1	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	498/514 (96%)	-0.15	4 (0%) 86 91	26, 39, 64, 100	0
2	B	517/519 (99%)	0.08	27 (5%) 27 39	27, 42, 85, 128	0
3	C	310/330 (93%)	0.03	18 (5%) 23 33	26, 46, 79, 109	0
All	All	1325/1363 (97%)	-0.02	49 (3%) 41 54	26, 42, 77, 128	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	476	ARG	8.8
3	C	182	SER	5.4
2	B	494	CYS	5.2
2	B	487	TRP	4.8
3	C	186	LEU	4.7
2	B	474	TYR	4.6
1	A	246	THR	4.4
2	B	483	LEU	4.0
2	B	518	GLU	3.7
2	B	489	GLY	3.6
2	B	479	LYS	3.6
3	C	178	ASN	3.5
3	C	183	ILE	3.4
2	B	460	ASN	3.4
2	B	488	ASP	3.3
2	B	495	SER	3.2
2	B	498	VAL	3.2
1	A	163	GLY	3.2
3	C	184	SER	3.1
2	B	504	SER	3.1
2	B	480	HIS	3.1
2	B	508	ARG	2.9
3	C	266	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	160	HIS	2.9
2	B	486	GLY	2.9
2	B	477	GLY	2.8
2	B	478	LYS	2.8
2	B	475	PHE	2.8
3	C	267	HIS	2.8
3	C	142	THR	2.6
2	B	493	ASP	2.6
1	A	245	ASN	2.5
3	C	35	PRO	2.5
3	C	180	ILE	2.5
2	B	52	LEU	2.5
3	C	181	GLU	2.4
2	B	517	LYS	2.4
3	C	316	TYR	2.4
2	B	473	GLN	2.3
2	B	457	TYR	2.2
3	C	36	LEU	2.2
1	A	483	GLN	2.2
3	C	150	ASN	2.2
2	B	491	HIS	2.2
3	C	270	ALA	2.1
3	C	179	LYS	2.1
3	C	176	TYR	2.1
2	B	458	MET	2.0
2	B	456	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	605	6/6	0.77	0.26	52,62,65,67	0
4	GOL	C	403	6/6	0.81	0.31	62,66,67,74	0
4	GOL	B	602	6/6	0.81	0.17	49,54,64,66	0
4	GOL	C	402	6/6	0.83	0.18	44,52,55,57	0
4	GOL	A	603	6/6	0.86	0.20	57,59,65,65	0
4	GOL	A	602	6/6	0.86	0.12	49,54,59,62	0
4	GOL	A	601	6/6	0.89	0.14	39,43,45,45	0
4	GOL	B	601	6/6	0.91	0.14	54,56,59,59	0
4	GOL	B	604	6/6	0.93	0.21	43,47,52,52	0
4	GOL	A	606	6/6	0.93	0.16	40,43,50,51	0
4	GOL	B	603	6/6	0.95	0.09	40,45,47,53	0
4	GOL	C	401	6/6	0.95	0.11	38,41,45,48	0
4	GOL	A	604	6/6	0.96	0.26	43,45,52,52	0
5	SO4	A	608	5/5	0.97	0.11	57,58,70,76	0
5	SO4	A	607	5/5	0.99	0.07	38,44,49,55	0
5	SO4	B	605	5/5	0.99	0.09	44,45,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.