



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:21 AM UTC

PDB ID : 6OYC / pdb_00006oyc
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 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

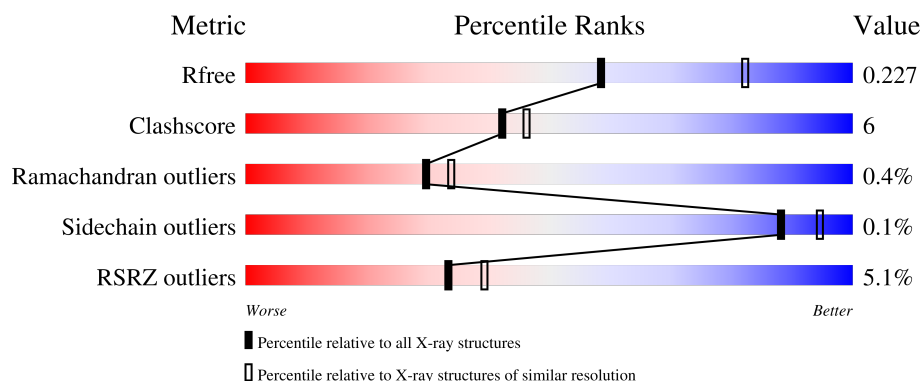
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 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	514	2% 87% 10% .
2	B	519	5% 85% 14%
3	C	330	9% 76% 17% 6%

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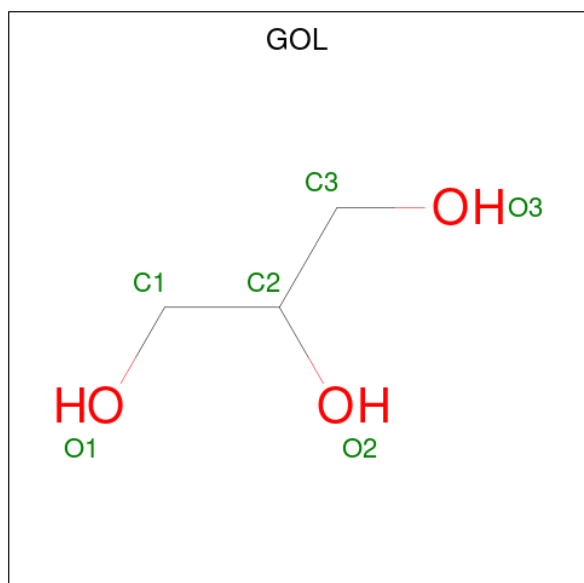
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Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASN	-	expression tag	UNP Q8DYM5
B	22	ILE	-	expression tag	UNP Q8DYM5
B	23	PRO	-	expression tag	UNP Q8DYM5
B	24	ASN	-	expression tag	UNP Q8DYM5
B	25	ASN	-	expression tag	UNP Q8DYM5

- 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 (CCD ID: GOL) (formula: C₃H₈O₃).



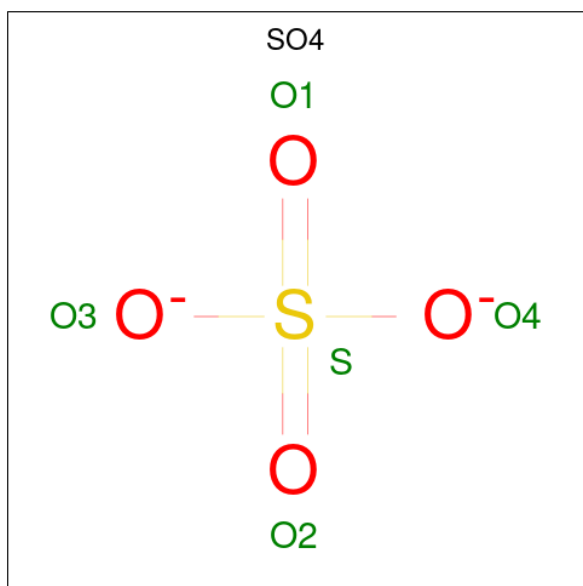
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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 (CCD ID: 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		

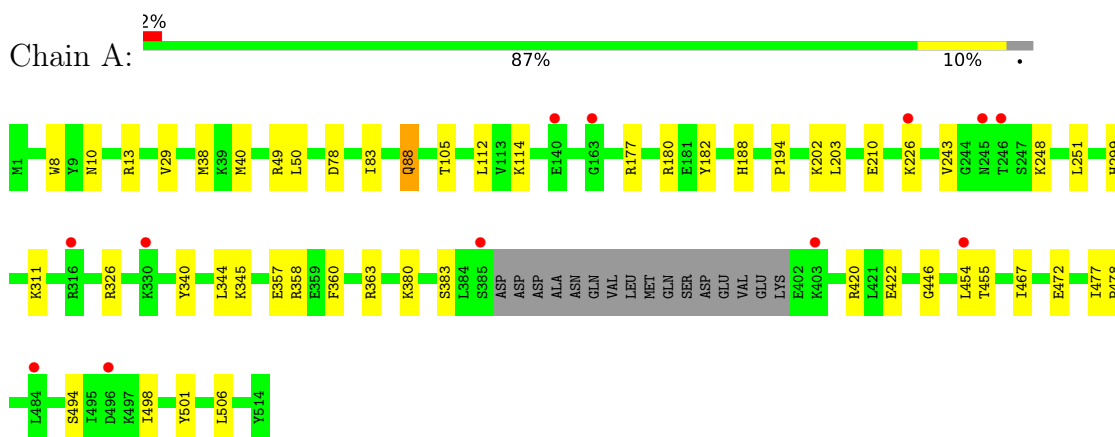
- Molecule 6 is water.

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

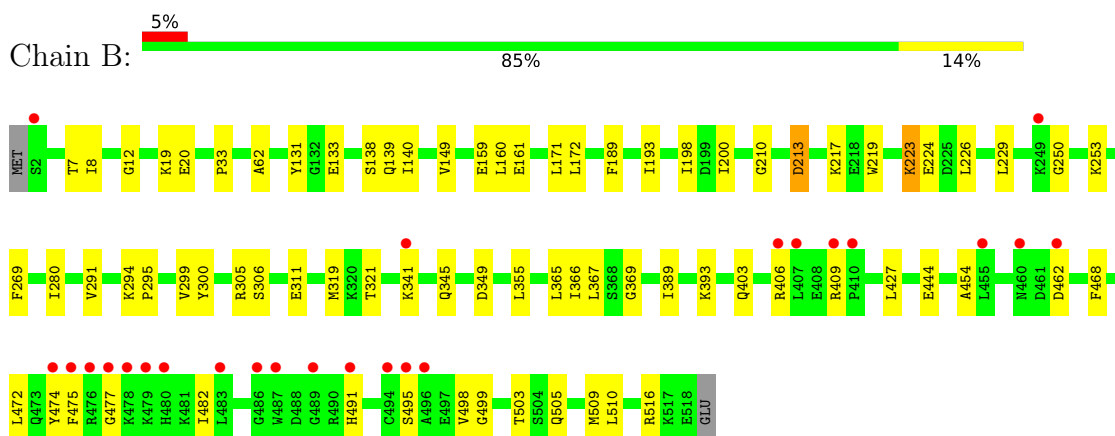
3 Residue-property plots

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.

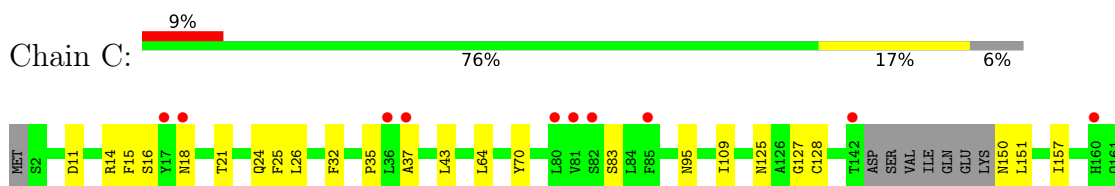
• Molecule 1: Glycosylation Associate Protein 1



• Molecule 2: Glycosylation Associate Protein 2



• Molecule 3: Glycosylation Associate Protein 3





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) 99.5 (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 0.183 , 0.227	Depositor DCC
R_{free} test set	2003 reflections (2.74%)	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)	0.36 , 40.1	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: SO4, 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	0.37	1/4246 (0.0%)	0.55	0/5744
2	B	0.40	2/4263 (0.0%)	0.54	2/5750 (0.0%)
3	C	0.36	0/2573	0.58	0/3492
All	All	0.38	3/11082 (0.0%)	0.55	2/14986 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	PRO	C-O	-7.61	1.18	1.25
1	A	88	GLN	C-O	-5.47	1.17	1.23
2	B	295	PRO	CA-C	-5.03	1.49	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	LYS	CA-C-N	5.24	123.48	119.66
2	B	294	LYS	C-N-CA	5.24	123.48	119.66

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	40	0
2	B	4163	0	4046	51	0
3	C	2514	0	2507	50	0
4	A	36	0	48	10	0
4	B	24	0	32	3	0
4	C	18	0	24	1	0
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	3	0
6	C	65	0	0	0	0
All	All	11323	0	10724	137	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 (137) 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)
2:B:366:ILE:CD1	2:B:509:MET:HE1	1.84	1.06
2:B:366:ILE:HD13	2:B:509:MET:HE1	1.41	1.02
1:A:38:MET:HE1	1:A:50:LEU:HD13	1.56	0.84
2:B:366:ILE:HD11	2:B:509:MET:HE1	1.61	0.82
3:C:157:ILE:HD11	3:C:164:LEU:HD22	1.67	0.77
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
1:A:40:MET:HE2	1:A:501:TYR:CD2	2.27	0.70
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:409:ARG:NH2	6:B:702:HOH:O	2.27	0.67
3:C:179:LYS:O	3:C:180:ILE:HG13	1.95	0.67
1:A:311:LYS:NZ	1:A:422:GLU:OE2	2.26	0.67
3:C:163:VAL:O	3:C:189:LYS:NZ	2.25	0.66
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:299:HIS:H	4:A:605:GOL:H11	1.65	0.62
1:A:420:ARG:HG3	6:A:703:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:462:ASP:OD2	2:B:462:ASP:N	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
2:B:193:ILE:HD11	2:B:280:ILE:HB	1.86	0.58
2:B:198:ILE:HD11	2:B:250:GLY:C	2.29	0.58
3:C:270:ALA:O	3:C:274:ILE:HD12	2.04	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
1:A:49:ARG:HD3	4:A:602:GOL:H11	1.88	0.55
3:C:184:SER:O	3:C:186:LEU:N	2.39	0.54
1:A:248:LYS:NZ	6:A:701:HOH:O	2.27	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
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
1:A:40:MET:HE2	1:A:501:TYR:HD2	1.74	0.53
2:B:140:ILE:HG23	2:B:172:LEU:HD13	1.90	0.53
2:B:366:ILE:HD11	2:B:509:MET:CE	2.37	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:OD1	3:C:11:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:202:LYS:NZ	1:A:210:GLU:OE2	2.32	0.49
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
3:C:179:LYS:C	3:C:181:GLU:H	2.16	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:167:LEU:HB2	3:C:190:VAL:HG21	1.95	0.47
3:C:186:LEU:HD23	3:C:187:GLN:N	2.28	0.47
3:C:268:LEU:HD23	3:C:273:GLN:CG	2.45	0.47
2:B:341:LYS:H	2:B:341:LYS:CE	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:HB3	1:A:345:LYS:HE2	1.74	0.46
1:A:49:ARG:NH2	6:A:705:HOH:O	2.39	0.46
3:C:32:PHE:C	3:C:32:PHE:CD1	2.93	0.46
2:B:160:LEU:HD13	2:B:171:LEU:HD21	1.97	0.45
1:A:38:MET:HE2	1:A:38:MET:HB2	1.54	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
1:A:40:MET:HE1	1:A:506:LEU:HD23	1.99	0.44
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
2:B:131:TYR:OH	2:B:133:GLU:OE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:LYS:O	3:C:181:GLU:HG2	2.17	0.44
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
3:C:178:ASN:C	3:C:179:LYS:HG3	2.44	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
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:7:THR:O	2:B:8:ILE:HD13	2.20	0.42
2:B:12:GLY:O	2:B:33:PRO:HD3	2.20	0.42
3:C:315:PRO:C	3:C:317:LEU:H	2.28	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
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:150:ASN:CG	3:C:151:LEU:H	2.27	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
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
2:B:19:LYS:NZ	6:B:710:HOH:O	2.50	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
2	B	515/519 (99%)	493 (96%)	18 (4%)	4 (1%)	16	17
3	C	306/330 (93%)	285 (93%)	20 (6%)	1 (0%)	36	43
All	All	1315/1363 (96%)	1261 (96%)	49 (4%)	5 (0%)	30	34

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%)	459 (100%)	1 (0%)	87	94
2	B	447/450 (99%)	447 (100%)	0	100	100
3	C	287/307 (94%)	287 (100%)	0	100	100
All	All	1194/1232 (97%)	1193 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	85	ASN
1	A	236	GLN
1	A	329	HIS
2	B	151	ASN
2	B	156	ASN
2	B	359	ASN
2	B	403	GLN
2	B	423	ASN
3	C	187	GLN
3	C	188	GLN
3	C	234	ASN
3	C	302	ASN
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 oligosaccharides 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	A	605	-	5,5,5	0.94	0	5,5,5	1.10	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	606	-	5,5,5	1.14	0	5,5,5	1.11	0
4	GOL	C	401	-	5,5,5	0.81	0	5,5,5	1.13	0
4	GOL	B	603	-	5,5,5	0.94	0	5,5,5	1.19	1 (20%)
5	SO4	B	605	-	4,4,4	0.18	0	6,6,6	0.20	0
4	GOL	C	402	-	5,5,5	1.22	0	5,5,5	0.77	0
4	GOL	B	602	-	5,5,5	1.04	0	5,5,5	1.13	0
4	GOL	A	601	-	5,5,5	1.11	1 (20%)	5,5,5	1.15	0
4	GOL	A	602	-	5,5,5	0.83	0	5,5,5	1.10	1 (20%)
5	SO4	A	608	-	4,4,4	0.27	0	6,6,6	0.24	0
4	GOL	C	403	-	5,5,5	0.86	0	5,5,5	1.05	0
4	GOL	B	604	-	5,5,5	1.00	0	5,5,5	1.16	0
4	GOL	A	604	-	5,5,5	1.05	1 (20%)	5,5,5	1.27	0
4	GOL	A	603	-	5,5,5	0.93	0	5,5,5	0.96	0
5	SO4	A	607	-	4,4,4	0.26	0	6,6,6	0.13	0
4	GOL	B	601	-	5,5,5	0.79	0	5,5,5	1.01	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	A	605	-	-	2/4/4/4	-
4	GOL	A	606	-	-	4/4/4/4	-
4	GOL	C	401	-	-	0/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
4	GOL	C	402	-	-	3/4/4/4	-
4	GOL	B	602	-	-	4/4/4/4	-
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	A	602	-	-	2/4/4/4	-
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	B	604	-	-	1/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	A	603	-	-	2/4/4/4	-
4	GOL	B	601	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	GOL	C3-C2	2.23	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	GOL	O2-C2	-2.04	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	GOL	C3-C2-C1	-2.11	104.07	111.80
4	A	605	GOL	C3-C2-C1	-2.04	104.33	111.80
4	B	603	GOL	C3-C2-C1	-2.02	104.39	111.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	GOL	O1-C1-C2-O2
4	A	602	GOL	O1-C1-C2-C3
4	A	603	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	A	605	GOL	O1-C1-C2-C3
4	A	606	GOL	O1-C1-C2-C3
4	A	606	GOL	C1-C2-C3-O3
4	B	602	GOL	O1-C1-C2-C3
4	B	603	GOL	C1-C2-C3-O3
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	A	604	GOL	O1-C1-C2-O2
4	A	606	GOL	O2-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
4	A	606	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
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	605	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	GOL	2	0
4	C	402	GOL	1	0
4	B	602	GOL	3	0
4	A	601	GOL	1	0
4	A	602	GOL	4	0
4	A	604	GOL	1	0
4	A	603	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%)	-0.13	12 (2%) 59 66	26, 39, 64, 100	0
2	B	517/519 (99%)	0.08	25 (4%) 35 41	27, 42, 85, 128	0
3	C	310/330 (93%)	0.29	30 (9%) 13 15	26, 46, 79, 109	0
All	All	1325/1363 (97%)	0.05	67 (5%) 33 39	26, 42, 77, 128	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	183	ILE	7.3
3	C	186	LEU	4.7
3	C	180	ILE	4.5
1	A	246	THR	4.2
3	C	181	GLU	4.1
3	C	184	SER	4.1
1	A	385	SER	3.8
2	B	487	TRP	3.6
3	C	182	SER	3.5
3	C	316	TYR	3.5
1	A	226	LYS	3.5
3	C	270	ALA	3.4
3	C	81	VAL	3.3
3	C	142	THR	3.2
2	B	341	LYS	3.2
2	B	494	CYS	3.2
2	B	474	TYR	3.2
3	C	80	LEU	3.1
3	C	318	THR	3.1
1	A	245	ASN	3.1
1	A	140	GLU	3.0
3	C	176	TYR	3.0
1	A	163	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	LYS	2.9
1	A	403	LYS	2.9
3	C	82	SER	2.9
2	B	477	GLY	2.9
2	B	410	PRO	2.9
2	B	409	ARG	2.9
2	B	496	ALA	2.9
3	C	160	HIS	2.8
2	B	455	LEU	2.8
2	B	480	HIS	2.8
2	B	476	ARG	2.7
3	C	36	LEU	2.7
3	C	18	ASN	2.6
3	C	274	ILE	2.6
2	B	460	ASN	2.6
3	C	37	ALA	2.5
3	C	269	THR	2.5
3	C	177	ILE	2.5
3	C	175	VAL	2.4
2	B	479	LYS	2.4
2	B	475	PHE	2.4
3	C	162	ASP	2.3
3	C	271	LYS	2.3
3	C	190	VAL	2.3
2	B	407	LEU	2.3
2	B	489	GLY	2.2
2	B	462	ASP	2.2
3	C	178	ASN	2.2
2	B	406	ARG	2.1
2	B	483	LEU	2.1
2	B	249	LYS	2.1
2	B	478	LYS	2.1
3	C	85	PHE	2.1
1	A	454	LEU	2.1
1	A	496	ASP	2.1
2	B	495	SER	2.1
1	A	484	LEU	2.1
3	C	185	GLN	2.1
2	B	486	GLY	2.1
2	B	491	HIS	2.0
3	C	17	TYR	2.0
3	C	189	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	2	SER	2.0
1	A	316	ARG	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 oligosaccharides 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(Å ²)	Q<0.9
4	GOL	C	403	6/6	0.78	0.16	62,66,67,74	0
4	GOL	B	602	6/6	0.79	0.13	49,54,64,66	0
4	GOL	A	605	6/6	0.80	0.15	52,62,65,67	0
4	GOL	B	604	6/6	0.82	0.16	43,47,52,52	0
4	GOL	A	603	6/6	0.82	0.13	57,59,65,65	0
4	GOL	A	602	6/6	0.83	0.12	49,54,59,62	0
4	GOL	C	402	6/6	0.86	0.14	44,52,55,57	0
4	GOL	B	601	6/6	0.87	0.12	54,56,59,59	0
4	GOL	A	604	6/6	0.88	0.14	43,45,52,52	0
4	GOL	A	606	6/6	0.90	0.17	40,43,50,51	0
4	GOL	A	601	6/6	0.90	0.12	39,43,45,45	0
4	GOL	C	401	6/6	0.93	0.08	38,41,45,48	0
5	SO4	A	608	5/5	0.93	0.13	57,58,70,76	0
4	GOL	B	603	6/6	0.95	0.08	40,45,47,53	0
5	SO4	A	607	5/5	0.97	0.12	38,44,49,55	0
5	SO4	B	605	5/5	0.98	0.09	44,45,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.