



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:17 PM BST

PDB ID : 5JOP
Title : Crystal structure of anti-glycan antibody Fab14.22 in complex with Streptococcus pneumoniae serotype 14 tetrasaccharide at 1.75 Å
Authors : Sarkar, A.; Irimia, A.; Teyton, L.; Wilson, I.A.
Deposited on : 2016-05-02
Resolution : 1.75 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

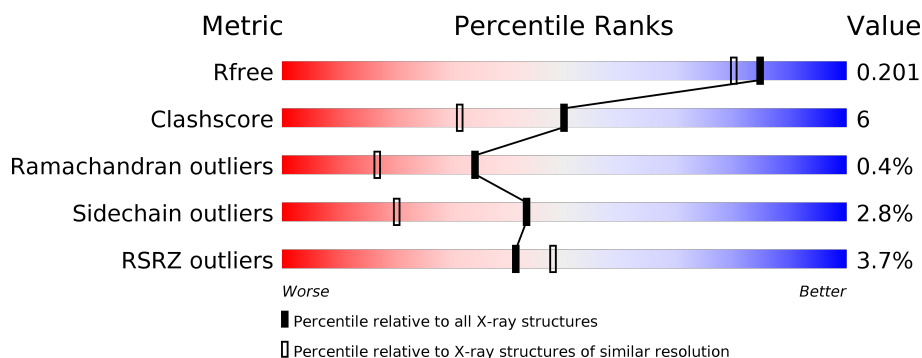
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	D	219	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
1	L	219	<div>2%</div> <div>91%</div> <div>8%</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	PO4	L	305	-	-	X	-
5	GOL	E	307	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8094 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.

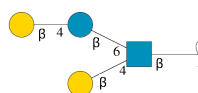
- Molecule 1 is a protein called Fab 14.22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	218	Total	C	N	O	S	0	17	0
			1828	1143	307	370	8			
1	L	218	Total	C	N	O	S	0	11	0
			1786	1123	302	354	7			

- Molecule 2 is a protein called Fab14.22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	208	Total	C	N	O	S	0	6	0
			1603	1019	258	319	7			
2	H	211	Total	C	N	O	S	0	3	0
			1626	1025	268	325	8			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	4	Total	C	N	O	0	0	0
			48	26	1	21			
3	B	4	Total	C	N	O	0	0	0
			48	26	1	21			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	L	1	Total	O	P	0	0
			5	4	1		
4	L	1	Total	O	P	0	0
			5	4	1		
4	L	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	270	Total	O	0	0
			270	270		
6	E	270	Total	O	0	0
			270	270		
6	L	261	Total	O	0	0
			261	261		
6	H	228	Total	O	0	0
			228	228		

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: Fab 14.22 light chain

Chain D:  86% 12% .



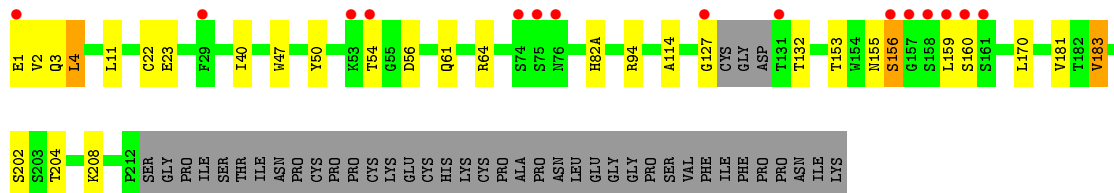
- Molecule 1: Fab 14.22 light chain

Chain L:  91% 8% .




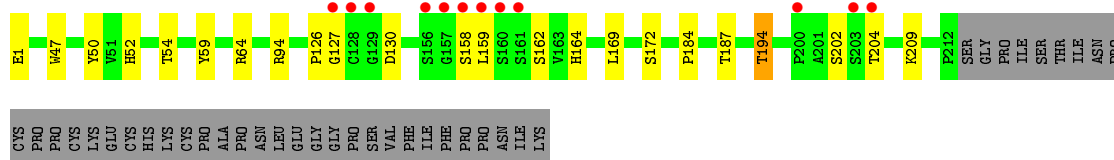
- Molecule 2: Fab14.22 heavy chain

Chain E:  71% 11% . 16%




- Molecule 2: Fab14.22 heavy chain

Chain H:  76% 9% 15%



- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  75% 25%

HA01
EGC2
GAL3
GAL4

- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

HA01
EGC2
GAL3
GAL4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.27Å 74.74Å 120.30Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	47.18 – 1.75 47.19 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.18-1.75) 96.9 (47.19-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.10_2155: 000)	Depositor
R, R_{free}	0.165 , 0.200 0.167 , 0.201	Depositor DCC
R_{free} test set	5339 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8094	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 6.37% 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: GAL, GOL, PO4, BGC, NAG

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	D	0.70	2/1877 (0.1%)	0.71	0/2548
1	L	0.69	0/1844	0.77	0/2503
2	E	0.66	0/1664	0.76	2/2278 (0.1%)
2	H	0.68	0/1670	0.75	0/2285
All	All	0.68	2/7055 (0.0%)	0.74	2/9614 (0.0%)

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	D	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	194[A]	CYS	CB-SG	-5.64	1.72	1.81
1	D	194[B]	CYS	CB-SG	-5.64	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	183	VAL	CG1-CB-CG2	9.30	125.78	110.90
2	E	183	VAL	CA-CB-CG1	5.54	119.22	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	156[B]	GLN	Peptide
1	D	157[B]	ASN	Mainchain,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	D	1828	0	1756	22	0
1	L	1786	0	1745	15	0
2	E	1603	0	1571	22	0
2	H	1626	0	1571	14	0
3	A	48	0	42	0	2
3	B	48	0	42	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	H	5	0	0	0	0
4	L	15	0	0	0	2
5	D	12	0	16	4	0
5	E	42	0	54	9	0
5	H	6	0	8	1	0
5	L	36	0	48	9	0
6	D	270	0	0	9	0
6	E	270	0	0	15	1
6	H	228	0	0	4	0
6	L	261	0	0	13	1
All	All	8094	0	6853	81	3

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 (81) 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:L:199:LYS:NZ	6:L:401:HOH:O	2.10	0.84
1:D:40:PRO:O	6:D:402:HOH:O	1.96	0.83
1:D:143[B]:ASP:OD2	6:D:401:HOH:O	1.96	0.83
2:E:155:ASN:ND2	6:E:403:HOH:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54[A]:THR:HG23	2:E:56:ASP:H	1.45	0.80
4:E:301:PO4:O2	6:E:401:HOH:O	2.01	0.76
2:H:126:PRO:O	6:H:401:HOH:O	2.03	0.76
5:E:303:GOL:O2	6:E:402:HOH:O	2.02	0.74
1:D:24:ARG:NE	1:D:70[B]:ASP:OD1	2.25	0.68
1:L:165:ASP:OD2	6:L:402:HOH:O	2.12	0.67
1:L:145[A]:ASN:OD1	5:L:310:GOL:O3	2.13	0.66
5:L:310:GOL:O2	6:L:403:HOH:O	2.13	0.65
2:E:54[A]:THR:HG21	6:E:550:HOH:O	1.96	0.65
1:D:54:ARG:HB2	5:D:306:GOL:H31	1.79	0.65
6:L:593:HOH:O	2:H:169:LEU:HD11	1.96	0.63
1:L:154:GLU:OE2	6:L:404:HOH:O	2.15	0.63
2:E:202:SER:O	2:E:204[B]:THR:HG23	1.99	0.62
2:H:54:THR:HG21	5:H:302:GOL:H31	1.84	0.60
2:H:127:GLY:HA3	6:H:589:HOH:O	2.03	0.59
2:H:1:GLU:HB3	6:H:434:HOH:O	2.02	0.59
2:E:159:LEU:HD11	6:E:403:HOH:O	2.04	0.58
2:H:194[B]:THR:HG22	2:H:209:LYS:HA	1.84	0.58
1:L:155:ARG:HH22	1:L:185:GLU:CD	2.07	0.58
5:L:312:GOL:O1	6:L:405:HOH:O	2.17	0.57
5:D:307:GOL:O3	6:D:404:HOH:O	2.18	0.56
2:E:82(A):HIS:ND1	5:E:304:GOL:H32	2.22	0.55
2:E:11:LEU:HD11	6:E:406:HOH:O	2.06	0.55
1:D:39:ARG:NH2	6:D:424:HOH:O	2.41	0.54
5:E:307:GOL:O2	5:L:313:GOL:H32	2.08	0.54
2:E:2[A]:VAL:HG11	6:E:577:HOH:O	2.08	0.54
1:D:105:GLU:OE2	6:D:403:HOH:O	2.17	0.53
6:L:628:HOH:O	2:H:169:LEU:HB3	2.08	0.53
2:H:64[B]:ARG:NH2	6:H:404:HOH:O	2.30	0.53
1:D:157[B]:ASN:CG	1:D:158:GLY:H	2.13	0.53
2:E:127:GLY:N	6:E:413:HOH:O	2.38	0.52
1:D:13[A]:VAL:HG22	1:D:17:ASP:HB2	1.91	0.52
1:D:37:LEU:HB2	1:D:47:LEU:HD11	1.93	0.51
2:H:202:SER:O	2:H:204:THR:HG23	2.10	0.51
1:L:197:THR:HG22	5:L:310:GOL:H12	1.91	0.51
1:D:103:LYS:NZ	6:D:420:HOH:O	2.37	0.51
2:E:114:ALA:O	6:E:406:HOH:O	2.19	0.51
5:E:302:GOL:O2	6:E:405:HOH:O	2.18	0.50
1:D:151:ASP:OD2	6:D:406:HOH:O	2.20	0.49
5:L:312:GOL:H31	2:H:164:HIS:ND1	2.26	0.49
1:L:39[A]:ARG:NH2	5:L:308:GOL:O1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:308:GOL:H2	1:L:3:LEU:HD13	1.96	0.48
1:D:203[B]:SER:OG	6:D:407:HOH:O	2.20	0.47
2:E:170:LEU:HD12	5:L:313:GOL:H31	1.96	0.47
2:E:159:LEU:HD13	2:E:181:VAL:HG21	1.97	0.47
5:E:307:GOL:O3	5:E:307:GOL:O1	2.28	0.47
2:E:40:ILE:HD13	5:E:308:GOL:H32	1.97	0.47
2:E:3:GLN:NE2	6:E:422:HOH:O	2.48	0.47
1:D:155:ARG:HD2	1:D:156[B]:GLN:O	2.16	0.46
2:E:159:LEU:HD21	6:E:403:HOH:O	2.15	0.46
2:E:61:GLN:HA	2:E:64:ARG:HG2	1.97	0.46
1:L:21[A]:ILE:CG2	6:L:428:HOH:O	2.63	0.46
1:L:21[A]:ILE:HG22	6:L:428:HOH:O	2.15	0.46
1:D:96:ARG:HB2	2:E:47:TRP:CG	2.52	0.45
1:L:63:ARG:NH2	6:L:414:HOH:O	2.36	0.45
1:D:34:GLU:HG2	1:D:49:TYR:HA	1.98	0.45
5:E:303:GOL:H11	6:E:578:HOH:O	2.17	0.45
1:D:63:ARG:HH11	1:D:63:ARG:HG2	1.82	0.44
5:L:311:GOL:O1	6:L:406:HOH:O	2.20	0.44
1:D:157[B]:ASN:ND2	2:H:59:TYR:O	2.48	0.44
2:E:4:LEU:HG	2:E:22:CYS:SG	2.57	0.44
1:D:54:ARG:H	5:D:306:GOL:H11	1.82	0.43
2:E:159:LEU:HD22	6:E:425:HOH:O	2.18	0.43
1:D:54:ARG:H	5:D:306:GOL:H31	1.83	0.43
1:D:2:VAL:HG21	1:D:93:TYR:CD1	2.53	0.43
1:D:6:GLN:HB3	6:D:412:HOH:O	2.18	0.43
1:L:96:ARG:HB2	2:H:47:TRP:CG	2.54	0.43
2:E:23:GLU:OE1	6:E:407:HOH:O	2.22	0.43
2:E:208:LYS:HE3	2:E:208:LYS:HB3	1.91	0.42
1:D:136:LEU:HD21	1:D:146[B]:VAL:HG22	2.00	0.42
1:L:21[B]:ILE:HG21	1:L:102:THR:HG21	2.02	0.42
1:L:61:ARG:CZ	1:L:79:GLU:HG3	2.50	0.42
1:L:181:LEU:O	6:L:407:HOH:O	2.21	0.42
2:E:153:THR:HG22	2:E:156:SER:HA	2.02	0.41
5:E:308:GOL:H12	6:L:536:HOH:O	2.21	0.41
2:H:184:PRO:HB2	2:H:187:THR:HG23	2.03	0.41
2:H:158:SER:O	2:H:159:LEU:HD23	2.21	0.40

All (3) 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)
3:A:3:GAL:O4	4:L:305:PO4:O1[3_455]	1.23	0.97
3:A:3:GAL:C6	4:L:305:PO4:O1[3_455]	2.09	0.11
6:E:470:HOH:O	6:L:541:HOH:O[4_455]	2.19	0.01

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	D	234/219 (107%)	226 (97%)	6 (3%)	2 (1%)	17	5
1	L	228/219 (104%)	223 (98%)	5 (2%)	0	100	100
2	E	210/249 (84%)	206 (98%)	2 (1%)	2 (1%)	15	4
2	H	212/249 (85%)	208 (98%)	4 (2%)	0	100	100
All	All	884/936 (94%)	863 (98%)	17 (2%)	4 (0%)	34	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	157[A]	ASN
1	D	157[B]	ASN
2	E	156	SER
2	E	160	SER

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	D	212/195 (109%)	207 (98%)	5 (2%)	49	26
1	L	206/195 (106%)	202 (98%)	4 (2%)	57	37
2	E	187/218 (86%)	181 (97%)	6 (3%)	39	16
2	H	187/218 (86%)	179 (96%)	8 (4%)	29	9
All	All	792/826 (96%)	769 (97%)	23 (3%)	43	19

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	63	ARG
1	D	157[A]	ASN
1	D	157[B]	ASN
1	D	175	MET
1	D	213	GLU
2	E	1	GLU
2	E	4	LEU
2	E	50	TYR
2	E	94	ARG
2	E	132	THR
2	E	183	VAL
1	L	56	SER
1	L	165	ASP
1	L	169	LYS
1	L	213	GLU
2	H	50	TYR
2	H	52	HIS
2	H	94	ARG
2	H	130	ASP
2	H	162	SER
2	H	172	SER
2	H	194[A]	THR
2	H	194[B]	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	1	3	15,15,15	1.42	2 (13%)	21,21,21	1.42	2 (9%)
3	BGC	A	2	3	11,11,12	0.79	0	15,15,17	1.96	4 (26%)
3	GAL	A	3	3	11,11,12	1.78	3 (27%)	15,15,17	3.74	6 (40%)
3	GAL	A	4	3	11,11,12	1.32	1 (9%)	15,15,17	1.40	3 (20%)
3	NAG	B	1	3	15,15,15	1.07	1 (6%)	21,21,21	1.13	2 (9%)
3	BGC	B	2	3	11,11,12	0.69	0	15,15,17	1.06	1 (6%)
3	GAL	B	3	3	11,11,12	0.96	0	15,15,17	1.22	2 (13%)
3	GAL	B	4	3	11,11,12	0.89	0	15,15,17	1.39	2 (13%)

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	NAG	A	1	3	-	2/6/26/26	0/1/1/1
3	BGC	A	2	3	-	2/2/19/22	0/1/1/1
3	GAL	A	3	3	-	0/2/19/22	0/1/1/1
3	GAL	A	4	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1	3	-	2/6/26/26	0/1/1/1
3	BGC	B	2	3	-	0/2/19/22	0/1/1/1
3	GAL	B	3	3	-	0/2/19/22	0/1/1/1
3	GAL	B	4	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3	GAL	O5-C5	4.02	1.51	1.43
3	A	3	GAL	O5-C1	2.95	1.48	1.43
3	A	1	NAG	C1-C2	2.48	1.55	1.52
3	B	1	NAG	O7-C7	-2.44	1.17	1.23
3	A	4	GAL	O5-C5	2.39	1.48	1.43
3	A	3	GAL	O4-C4	2.12	1.48	1.43
3	A	1	NAG	C8-C7	2.00	1.54	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	GAL	C6-C5-C4	-7.93	94.43	113.00
3	A	3	GAL	O4-C4-C3	6.59	125.59	110.35
3	A	3	GAL	C1-O5-C5	5.78	120.02	112.19
3	A	3	GAL	O4-C4-C5	-5.14	96.53	109.30
3	A	2	BGC	C1-O5-C5	4.38	118.12	112.19
3	A	3	GAL	O5-C5-C6	4.32	113.98	107.20
3	A	3	GAL	O6-C6-C5	-4.03	97.46	111.29
3	B	4	GAL	C1-C2-C3	3.92	114.48	109.67
3	A	1	NAG	C4-C3-C2	-3.27	105.55	110.34
3	A	2	BGC	O6-C6-C5	-3.07	100.77	111.29
3	A	1	NAG	C1-C2-N2	-3.06	107.19	110.73
3	A	4	GAL	C1-O5-C5	2.89	116.11	112.19
3	B	1	NAG	O1-C1-C2	2.88	115.20	109.22
3	A	2	BGC	O4-C4-C5	-2.68	102.64	109.30
3	A	4	GAL	C2-C3-C4	2.53	115.27	110.89
3	A	2	BGC	O5-C5-C4	-2.46	104.84	110.83
3	B	3	GAL	O6-C6-C5	-2.35	103.23	111.29
3	B	3	GAL	O2-C2-C1	-2.28	104.48	109.15
3	B	2	BGC	C6-C5-C4	2.22	118.19	113.00
3	B	4	GAL	C1-O5-C5	2.20	115.18	112.19
3	A	4	GAL	O3-C3-C2	-2.16	105.85	109.99
3	B	1	NAG	C4-C3-C2	-2.09	107.28	110.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2	BGC	O5-C5-C6-O6
3	A	2	BGC	C4-C5-C6-O6
3	B	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C3-C2-N2-C7
3	A	1	NAG	C1-C2-N2-C7
3	B	1	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	GAL	0	2

5.6 Ligand geometry [i](#)

22 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	PO4	L	307	-	4,4,4	0.85	0	6,6,6	0.36	0
4	PO4	D	305	-	4,4,4	0.75	0	6,6,6	0.54	0
4	PO4	L	306	-	4,4,4	0.81	0	6,6,6	0.48	0
5	GOL	L	308	-	5,5,5	0.35	0	5,5,5	0.46	0
5	GOL	D	306	-	5,5,5	0.33	0	5,5,5	0.28	0
5	GOL	E	304	-	5,5,5	0.43	0	5,5,5	0.22	0
5	GOL	E	308	-	5,5,5	0.32	0	5,5,5	0.45	0
5	GOL	H	302	-	5,5,5	0.39	0	5,5,5	0.22	0
5	GOL	L	313	-	5,5,5	0.32	0	5,5,5	0.30	0
5	GOL	E	306	2	5,5,5	0.63	0	5,5,5	1.22	1 (20%)
4	PO4	E	301	-	4,4,4	0.63	0	6,6,6	1.73	2 (33%)
5	GOL	L	311	-	5,5,5	0.50	0	5,5,5	0.15	0
5	GOL	E	307	-	5,5,5	0.28	0	5,5,5	0.16	0
4	PO4	L	305	-	4,4,4	1.80	1 (25%)	6,6,6	0.87	0
5	GOL	E	303	-	5,5,5	0.47	0	5,5,5	0.63	0
5	GOL	E	305	-	5,5,5	0.39	0	5,5,5	1.11	0
5	GOL	E	302	-	5,5,5	0.45	0	5,5,5	0.80	0
5	GOL	L	312	-	5,5,5	0.34	0	5,5,5	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	L	309	-	5,5,5	0.43	0	5,5,5	1.65	1 (20%)
5	GOL	D	307	-	5,5,5	0.38	0	5,5,5	0.68	0
4	PO4	H	301	-	4,4,4	0.83	0	6,6,6	0.46	0
5	GOL	L	310	-	5,5,5	0.42	0	5,5,5	0.31	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
5	GOL	L	311	-	-	0/4/4/4	-
5	GOL	E	305	-	-	1/4/4/4	-
5	GOL	E	302	-	-	4/4/4/4	-
5	GOL	L	308	-	-	3/4/4/4	-
5	GOL	E	308	-	-	1/4/4/4	-
5	GOL	L	312	-	-	3/4/4/4	-
5	GOL	D	306	-	-	4/4/4/4	-
5	GOL	E	304	-	-	0/4/4/4	-
5	GOL	E	303	-	-	4/4/4/4	-
5	GOL	L	309	-	-	2/4/4/4	-
5	GOL	H	302	-	-	1/4/4/4	-
5	GOL	D	307	-	-	0/4/4/4	-
5	GOL	E	307	-	-	2/4/4/4	-
5	GOL	L	310	-	-	2/4/4/4	-
5	GOL	L	313	-	-	0/4/4/4	-
5	GOL	E	306	2	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	305	PO4	P-O1	3.15	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	309	GOL	C3-C2-C1	-3.46	98.27	111.70
4	E	301	PO4	O4-P-O1	-2.60	101.37	110.89
4	E	301	PO4	O4-P-O3	2.39	115.63	107.97
5	E	306	GOL	O3-C3-C2	-2.04	100.41	110.20

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	306	GOL	O1-C1-C2-C3
5	D	306	GOL	C1-C2-C3-O3
5	E	303	GOL	O1-C1-C2-C3
5	E	302	GOL	O1-C1-C2-C3
5	E	302	GOL	C1-C2-C3-O3
5	E	302	GOL	O2-C2-C3-O3
5	L	312	GOL	O1-C1-C2-C3
5	L	309	GOL	O1-C1-C2-C3
5	L	310	GOL	C1-C2-C3-O3
5	E	302	GOL	O1-C1-C2-O2
5	L	308	GOL	C1-C2-C3-O3
5	E	306	GOL	C1-C2-C3-O3
5	E	307	GOL	O1-C1-C2-C3
5	E	303	GOL	C1-C2-C3-O3
5	E	305	GOL	O1-C1-C2-C3
5	D	306	GOL	O1-C1-C2-O2
5	D	306	GOL	O2-C2-C3-O3
5	E	306	GOL	O2-C2-C3-O3
5	E	303	GOL	O1-C1-C2-O2
5	E	303	GOL	O2-C2-C3-O3
5	L	312	GOL	O1-C1-C2-O2
5	L	310	GOL	O2-C2-C3-O3
5	L	312	GOL	C1-C2-C3-O3
5	L	308	GOL	O2-C2-C3-O3
5	L	309	GOL	O1-C1-C2-O2
5	E	308	GOL	O2-C2-C3-O3
5	H	302	GOL	O1-C1-C2-O2
5	E	307	GOL	O1-C1-C2-O2
5	L	308	GOL	O1-C1-C2-C3

There are no ring outliers.

15 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	308	GOL	1	0
5	D	306	GOL	3	0
5	E	304	GOL	1	0
5	E	308	GOL	3	0
5	H	302	GOL	1	0
5	L	313	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301	PO4	1	0
5	L	311	GOL	1	0
5	E	307	GOL	2	0
4	L	305	PO4	0	2
5	E	303	GOL	2	0
5	E	302	GOL	1	0
5	L	312	GOL	2	0
5	D	307	GOL	1	0
5	L	310	GOL	3	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	D	218/219 (99%)	-0.25	1 (0%) 91 93	16, 25, 44, 80	0
1	L	218/219 (99%)	-0.05	4 (1%) 68 76	15, 25, 45, 78	0
2	E	208/249 (83%)	0.21	15 (7%) 15 20	18, 27, 47, 75	0
2	H	211/249 (84%)	-0.06	12 (5%) 23 29	16, 26, 54, 74	0
All	All	855/936 (91%)	-0.04	32 (3%) 41 48	15, 26, 49, 80	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	159	LEU	6.3
2	H	156	SER	5.4
2	H	158	SER	5.3
2	H	128	CYS	5.3
2	E	156	SER	5.2
2	H	159	LEU	4.9
2	H	157	GLY	4.8
2	E	158	SER	4.4
2	E	131	THR	4.3
2	E	161	SER	4.2
2	H	160	SER	4.1
1	L	212	ASN	3.8
2	H	161	SER	3.0
2	H	127	GLY	3.0
2	H	129	GLY	3.0
1	D	157[A]	ASN	2.8
2	E	1	GLU	2.7
1	L	157	ASN	2.6
2	E	160	SER	2.6
2	E	157	GLY	2.5
2	H	204	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	74	SER	2.4
2	E	127	GLY	2.4
2	H	200	PRO	2.4
2	E	53	LYS	2.4
1	L	213	GLU	2.4
2	E	75	SER	2.2
2	H	203	SER	2.2
2	E	29	PHE	2.2
2	E	76	ASN	2.1
2	E	54[A]	THR	2.1
1	L	182	THR	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](#)

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
3	GAL	A	3	11/12	0.79	0.16	33,40,66,67	0
3	BGC	A	2	11/12	0.95	0.09	26,29,41,47	0
3	NAG	A	1	15/15	0.96	0.09	24,27,31,32	0
3	GAL	B	3	11/12	0.97	0.10	25,31,36,37	0
3	NAG	B	1	15/15	0.97	0.06	18,20,22,22	0
3	BGC	B	2	11/12	0.97	0.06	19,23,27,33	0
3	GAL	A	4	11/12	0.98	0.06	21,24,26,26	0
3	GAL	B	4	11/12	0.99	0.07	16,18,20,24	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. 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
5	GOL	E	307	6/6	0.30	0.62	84,86,87,88	0
5	GOL	E	306	6/6	0.74	0.24	38,45,48,49	0
4	PO4	L	305	5/5	0.76	0.21	48,48,56,56	0
5	GOL	L	313	6/6	0.78	0.21	77,78,79,80	0
5	GOL	D	306	6/6	0.78	0.25	75,76,76,79	0
5	GOL	H	302	6/6	0.79	0.13	55,57,57,57	0
5	GOL	E	304	6/6	0.81	0.22	65,67,67,71	0
5	GOL	L	311	6/6	0.83	0.36	59,60,65,66	0
5	GOL	L	312	6/6	0.83	0.17	52,53,57,60	0
5	GOL	E	308	6/6	0.84	0.18	44,53,54,54	0
4	PO4	H	301	5/5	0.84	0.24	104,104,104,105	0
5	GOL	L	310	6/6	0.84	0.18	50,56,57,60	0
4	PO4	L	307	5/5	0.85	0.19	87,88,89,90	0
4	PO4	L	306	5/5	0.87	0.18	75,77,79,80	0
5	GOL	D	307	6/6	0.87	0.16	65,66,68,70	0
5	GOL	E	303	6/6	0.89	0.30	47,54,56,57	0
5	GOL	L	308	6/6	0.91	0.21	46,52,54,58	0
4	PO4	E	301	5/5	0.91	0.15	46,47,53,56	0
5	GOL	L	309	6/6	0.93	0.10	26,29,31,32	0
4	PO4	D	305	5/5	0.94	0.22	55,61,63,64	0
5	GOL	E	302	6/6	0.95	0.11	26,35,40,48	0
5	GOL	E	305	6/6	0.95	0.15	21,27,36,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.