



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:45 PM GMT

PDB ID : 4W4O
Title : High-resolution crystal structure of Fc bound to its human receptor Fc-gamma-RI
Authors : Caaveiro, J.M.M.; Kiyoshi, M.; Tsumoto, K.
Deposited on : 2014-08-15
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

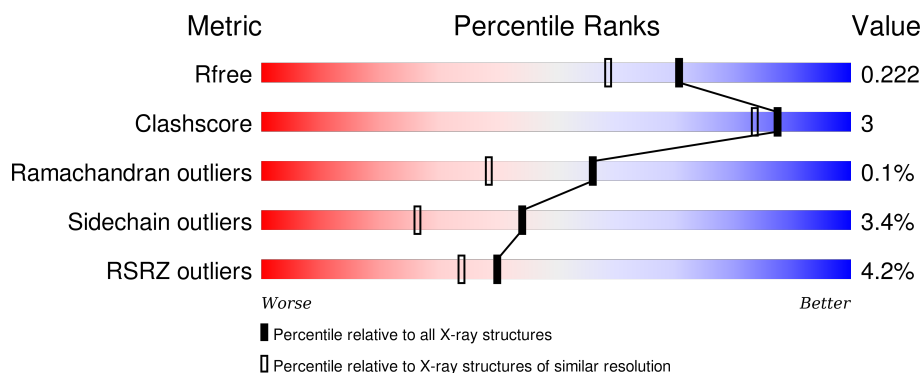
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	224	<div> <div>9%</div> <div>89%</div> <div>6%</div> <div>•</div> </div>
1	B	224	<div> <div>9%</div> <div>86%</div> <div>6%</div> <div>•</div> <div>7%</div> </div>
2	C	280	<div> <div>9%</div> <div>77%</div> <div>13%</div> <div>•</div> <div>8%</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
10	GOL	B	513	-	-	-	X
7	GAL	A	509	-	-	-	X
7	GAL	B	509	-	-	-	X
9	ACT	A	516	-	-	-	X
9	ACT	A	517	-	-	-	X
9	ACT	B	512	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6420 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	3	0
			1728	1103	291	328	6			
1	B	209	Total	C	N	O	S	0	3	0
			1682	1073	282	321	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ALA	SER	conflict	UNP P01857
B	444	ALA	SER	conflict	UNP P01857

- Molecule 2 is a protein called High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	259	Total	C	N	O	S	0	4	0
			2064	1310	356	387	11			

There are 25 discrepancies between the modelled and reference sequences:

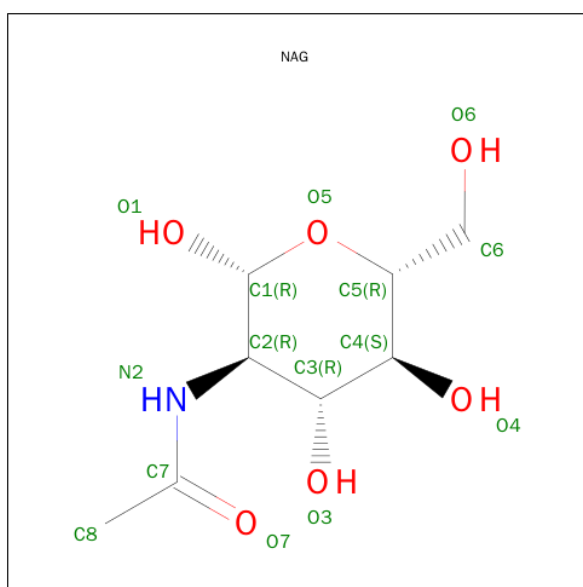
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	PRO	THR	engineered mutation	UNP P12314
C	25	LYS	THR	engineered mutation	UNP P12314
C	38	SER	THR	engineered mutation	UNP P12314
C	46	PRO	LEU	engineered mutation	UNP P12314
C	63	ILE	THR	engineered mutation	UNP P12314
C	69	THR	SER	engineered mutation	UNP P12314
C	71	HIS	ARG	engineered mutation	UNP P12314
C	77	GLU	VAL	engineered mutation	UNP P12314
C	78	ASP	ASN	engineered mutation	UNP P12314
C	100	VAL	ILE	engineered mutation	UNP P12314
C	114	LEU	PHE	engineered mutation	UNP P12314
C	160	MET	ILE	engineered mutation	UNP P12314

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Chain	Residue	Modelled	Actual	Comment	Reference
C	163	SER	ASN	engineered mutation	UNP P12314
C	195	THR	ASN	engineered mutation	UNP P12314
C	206	THR	ASN	engineered mutation	UNP P12314
C	207	PRO	LEU	engineered mutation	UNP P12314
C	240	ASP	ASN	engineered mutation	UNP P12314
C	283	HIS	LEU	engineered mutation	UNP P12314
C	285	GLN	LEU	engineered mutation	UNP P12314
C	290	HIS	-	expression tag	UNP P12314
C	291	HIS	-	expression tag	UNP P12314
C	292	HIS	-	expression tag	UNP P12314
C	293	HIS	-	expression tag	UNP P12314
C	294	HIS	-	expression tag	UNP P12314
C	295	HIS	-	expression tag	UNP P12314

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



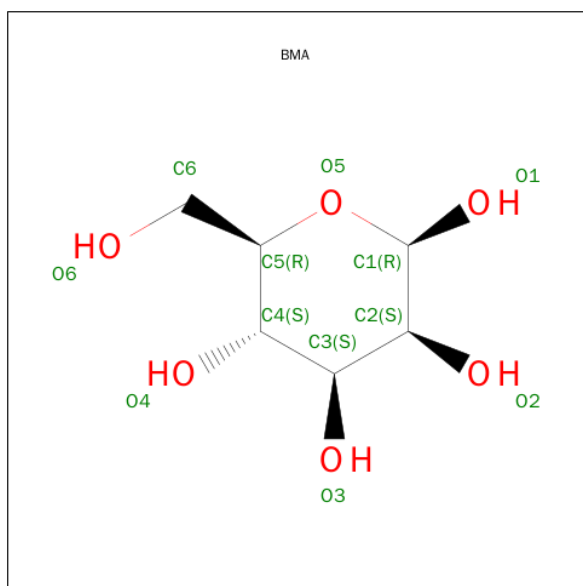
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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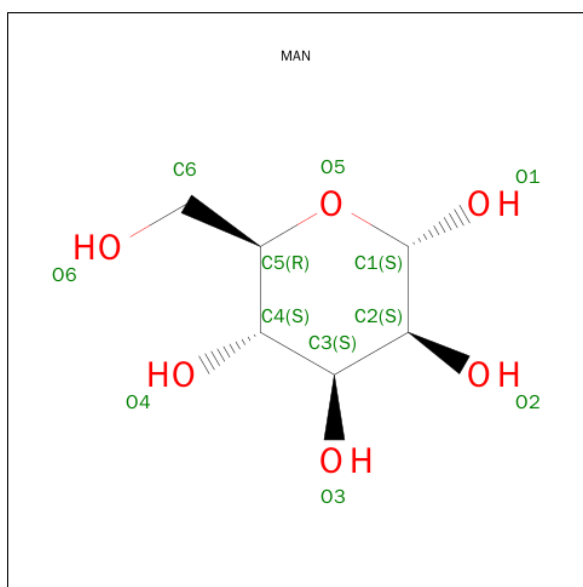
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



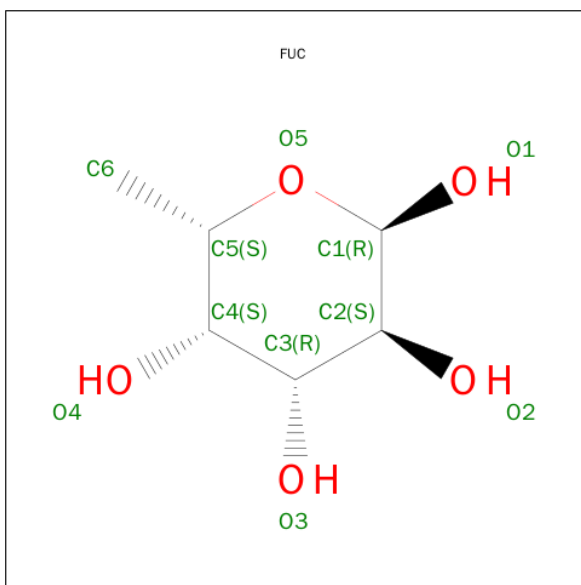
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



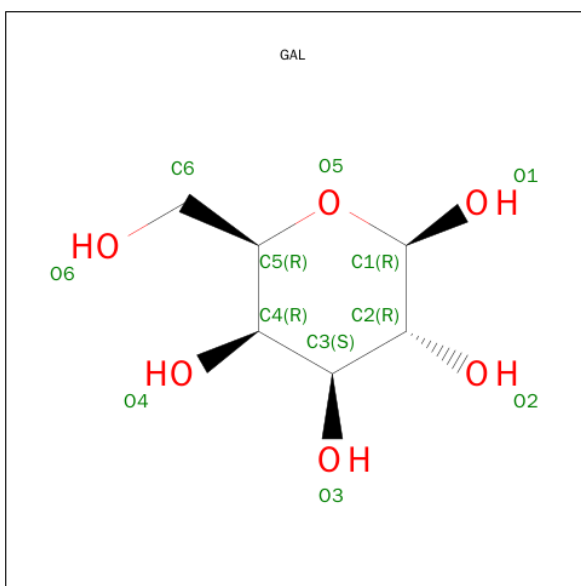
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).

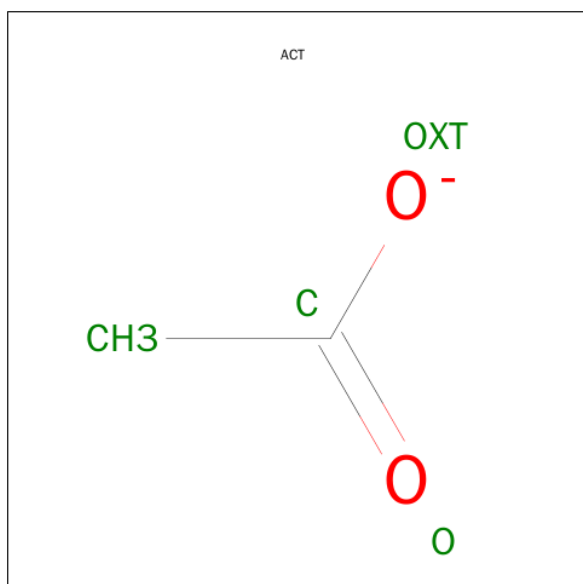


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Zn	0	0
			2	2		
8	A	3	Total	Zn	0	0
			3	3		
8	C	1	Total	Zn	0	0
			1	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



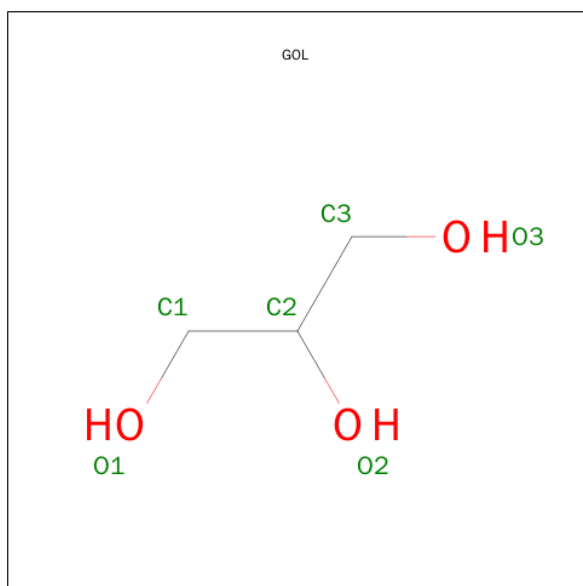
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

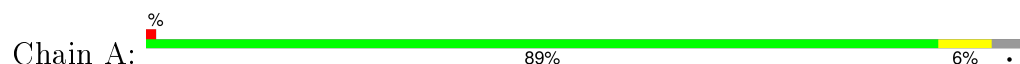
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	219	Total	O	0	3
			222	222		
11	B	178	Total	O	0	2
			180	180		
11	C	169	Total	O	0	1
			170	170		

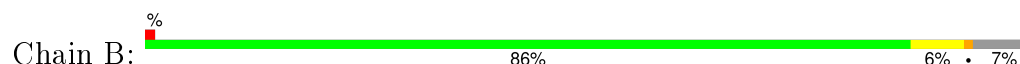
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

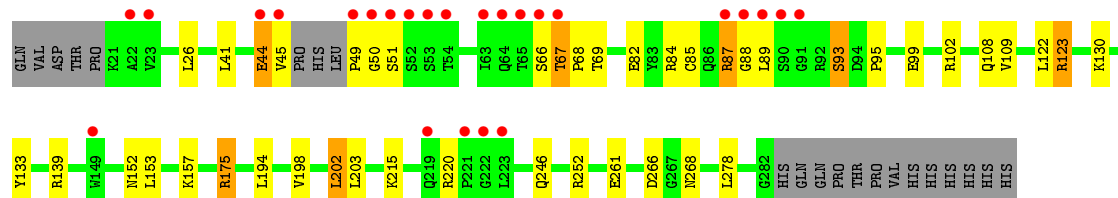
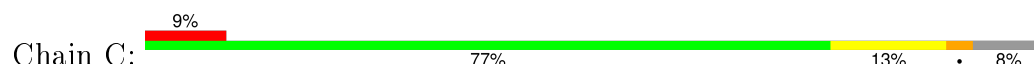
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region



- Molecule 2: High affinity immunoglobulin gamma Fc receptor I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.98 Å 126.50 Å 71.61 Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	39.70 – 1.80 37.59 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.70-1.80) 98.5 (37.59-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.173 , 0.215 0.184 , 0.222	Depositor DCC
R_{free} test set	4800 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 95656 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6420	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ZN, BMA, NAG, GAL, FUC, ACT, MAN

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	1.07	1/1785 (0.1%)	1.02	6/2432 (0.2%)
1	B	0.99	3/1737 (0.2%)	0.89	0/2367
2	C	0.97	1/2125 (0.0%)	1.05	10/2881 (0.3%)
All	All	1.01	5/5647 (0.1%)	1.00	16/7680 (0.2%)

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	B	0	1
2	C	0	6
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	SER	CB-OG	-8.10	1.31	1.42
2	C	99	GLU	CD-OE1	6.65	1.32	1.25
1	B	293	GLU	CD-OE1	5.85	1.32	1.25
1	B	381	TRP	CZ3-CH2	5.11	1.48	1.40
1	B	267	SER	CB-OG	-5.09	1.35	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	175	ARG	NE-CZ-NH2	10.18	125.39	120.30
2	C	266	ASP	CB-CG-OD1	8.02	125.52	118.30
2	C	175	ARG	NE-CZ-NH1	-7.28	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	139	ARG	NE-CZ-NH1	7.25	123.93	120.30
2	C	261	GLU	OE1-CD-OE2	6.99	131.69	123.30
2	C	194	LEU	CA-CB-CG	-6.24	100.95	115.30
2	C	278	LEU	CA-CB-CG	6.19	129.53	115.30
1	A	265	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	416	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	C	139	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	416	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	C	102	ARG	NE-CZ-NH2	5.66	123.13	120.30
2	C	123	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	388	GLU	N-CA-C	-5.50	96.15	111.00
1	A	294	GLU	OE1-CD-OE2	5.23	129.58	123.30
1	A	428	MET	CG-SD-CE	-5.09	92.06	100.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	235	LEU	Peptide
2	C	220	ARG	Peptide
2	C	44	GLU	Peptide
2	C	49	PRO	Peptide
2	C	50	GLY	Peptide
2	C	66	SER	Peptide
2	C	93	SER	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	1728	0	1709	4	0
1	B	1682	0	1659	9	0
2	C	2064	0	2046	18	0
3	A	56	0	48	0	0
3	B	56	0	48	0	0
3	C	56	0	49	0	0
4	A	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	8	0	0
4	C	11	0	9	0	0
5	A	22	0	18	0	0
5	B	22	0	18	0	0
5	C	33	0	28	0	0
6	A	10	0	10	0	0
6	B	10	0	10	0	0
7	A	11	0	9	0	0
7	B	11	0	10	1	0
8	A	3	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
9	A	24	0	18	1	0
9	B	4	0	3	0	0
9	C	8	0	6	0	0
10	A	6	0	8	0	0
10	B	6	0	8	1	0
11	A	222	0	0	0	0
11	B	180	0	0	1	1
11	C	170	0	0	2	1
All	All	6420	0	5730	30	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 3.

All (30) 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:C:67:THR:HG22	2:C:68:PRO:HD2	1.60	0.81
1:B:246:LYS:HG3	7:B:509:GAL:O4	1.97	0.65
1:A:355:ARG:HA	1:A:358:LEU:HD22	1.83	0.60
2:C:109:VAL:HG12	2:C:122:LEU:HD23	1.84	0.59
1:B:285:HIS:ND1	11:B:602:HOH:O	2.33	0.56
1:B:386:GLN:HA	1:B:386:GLN:HE21	1.71	0.55
1:B:355:ARG:HA	1:B:358:LEU:HD22	1.88	0.55
2:C:67:THR:CG2	2:C:68:PRO:HD2	2.34	0.53
2:C:26:LEU:CD2	2:C:41:LEU:HG	2.39	0.52
1:B:242:LEU:HD11	1:B:259[A]:VAL:CG1	2.41	0.50
2:C:130:LYS:NZ	11:C:404[A]:HOH:O	2.44	0.49
2:C:152:ASN:ND2	11:C:401:HOH:O	2.30	0.48
2:C:51:SER:O	2:C:87:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:O	9:A:514:ACT:H3	2.15	0.47
1:B:236:GLY:HA2	2:C:133:TYR:CD1	2.50	0.47
2:C:67:THR:HG22	2:C:68:PRO:CD	2.37	0.46
2:C:85:CYS:N	2:C:93:SER:OG	2.37	0.46
2:C:215:LYS:HG3	2:C:215:LYS:O	2.16	0.45
1:A:347[B]:GLN:HB3	1:A:349:TYR:CE2	2.52	0.45
1:B:242:LEU:HD11	1:B:259[A]:VAL:HG12	1.98	0.45
1:B:406:LEU:HD12	1:B:406:LEU:C	2.37	0.44
2:C:122:LEU:O	2:C:152:ASN:HB2	2.18	0.44
2:C:41:LEU:HD12	2:C:41:LEU:N	2.33	0.44
2:C:108:GLN:OE1	2:C:123:ARG:HD3	2.19	0.43
1:A:382:GLU:HG2	1:A:424:SER:HB2	2.01	0.42
2:C:198:VAL:CG2	2:C:202:LEU:HD22	2.51	0.41
2:C:84:ARG:NH1	2:C:93:SER:O	2.54	0.41
2:C:82:GLU:HG3	2:C:95:PRO:HB2	2.02	0.40
1:B:399:ASP:OD2	10:B:513:GOL:H31	2.21	0.40
2:C:153:LEU:HD23	2:C:153:LEU:HA	1.88	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)
11:B:725:HOH:O	11:C:549:HOH:O[4_546]	2.18	0.02

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	216/224 (96%)	214 (99%)	2 (1%)	0	100	100
1	B	210/224 (94%)	206 (98%)	4 (2%)	0	100	100
2	C	259/280 (92%)	250 (96%)	8 (3%)	1 (0%)	39	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	685/728 (94%)	670 (98%)	14 (2%)	1 (0%)	56 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	88	GLY

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	201/206 (98%)	198 (98%)	3 (2%)	72 62
1	B	197/206 (96%)	192 (98%)	5 (2%)	55 39
2	C	232/249 (93%)	219 (94%)	13 (6%)	26 10
All	All	630/661 (95%)	609 (97%)	21 (3%)	44 27

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LYS
1	A	358	LEU
1	A	438	GLN
1	B	235	LEU
1	B	245	PRO
1	B	344	ARG
1	B	358	LEU
1	B	386	GLN
2	C	44	GLU
2	C	45	VAL
2	C	67	THR
2	C	69	THR
2	C	87	ARG
2	C	89	LEU
2	C	157	LYS

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Mol	Chain	Res	Type
2	C	175	ARG
2	C	202	LEU
2	C	203	LEU
2	C	246	GLN
2	C	252	ARG
2	C	268	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	434	ASN
1	B	315	ASN
1	B	386	GLN
2	C	42	HIS
2	C	55	GLN
2	C	71	HIS
2	C	97	GLN
2	C	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

23 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	501	1,3,6	14,14,15	1.07	0	15,19,21	2.35	5 (33%)
3	NAG	A	502	3,4	14,14,15	1.37	2 (14%)	15,19,21	1.44	3 (20%)
5	MAN	A	504	3,4	11,11,12	0.84	1 (9%)	14,15,17	1.76	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	505	5,7	14,14,15	0.86	1 (7%)	15,19,21	1.07	1 (6%)
5	MAN	A	506	3,4	11,11,12	0.87	0	14,15,17	2.05	4 (28%)
3	NAG	A	507	5	14,14,15	0.74	0	15,19,21	1.26	2 (13%)
6	FUC	A	508	3	10,10,11	1.09	1 (10%)	14,14,16	2.18	6 (42%)
7	GAL	A	509	3	11,11,12	2.23	5 (45%)	14,15,17	2.94	7 (50%)
3	NAG	B	501	1,3,6	14,14,15	1.34	4 (28%)	15,19,21	1.06	0
3	NAG	B	502	3,4	14,14,15	0.94	0	15,19,21	1.46	4 (26%)
5	MAN	B	504	3,4	11,11,12	1.07	0	14,15,17	2.15	5 (35%)
3	NAG	B	505	5,7	14,14,15	0.91	0	15,19,21	1.19	2 (13%)
5	MAN	B	506	3,4	11,11,12	1.10	0	14,15,17	1.73	5 (35%)
3	NAG	B	507	5	14,14,15	0.65	0	15,19,21	1.61	4 (26%)
6	FUC	B	508	3	10,10,11	0.98	1 (10%)	14,14,16	2.48	4 (28%)
7	GAL	B	509	3	11,11,12	1.26	1 (9%)	14,15,17	2.57	4 (28%)
3	NAG	C	301	3,2	14,14,15	0.77	0	15,19,21	1.26	2 (13%)
3	NAG	C	302	3	14,14,15	0.64	0	15,19,21	2.74	6 (40%)
3	NAG	C	303	3,2	14,14,15	0.91	1 (7%)	15,19,21	1.65	2 (13%)
3	NAG	C	304	3,4	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
5	MAN	C	306	5,4	11,11,12	1.14	0	14,15,17	1.57	4 (28%)
5	MAN	C	307	5	11,11,12	1.39	2 (18%)	14,15,17	3.60	8 (57%)
5	MAN	C	308	5	11,11,12	0.98	0	14,15,17	3.45	6 (42%)

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	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
5	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	5,7	-	0/6/23/26	0/1/1/1
5	MAN	A	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	507	5	-	0/6/23/26	0/1/1/1
6	FUC	A	508	3	-	0/0/17/20	0/1/1/1
7	GAL	A	509	3	-	0/2/19/22	0/1/1/1
3	NAG	B	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
5	MAN	B	504	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	505	5,7	-	0/6/23/26	0/1/1/1
5	MAN	B	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	507	5	-	0/6/23/26	0/1/1/1
6	FUC	B	508	3	-	0/0/17/20	0/1/1/1
7	GAL	B	509	3	-	0/2/19/22	0/1/1/1
3	NAG	C	301	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	302	3	-	0/6/23/26	0/1/1/1
3	NAG	C	303	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	304	3,4	-	0/6/23/26	0/1/1/1
5	MAN	C	306	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	307	5	-	0/2/19/22	0/1/1/1
5	MAN	C	308	5	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	O5-C1	-4.10	1.36	1.43
7	A	509	GAL	O3-C3	-4.01	1.33	1.43
5	C	307	MAN	O5-C1	-3.19	1.38	1.43
3	B	501	NAG	O5-C1	-2.62	1.39	1.43
3	A	505	NAG	O5-C5	-2.38	1.38	1.43
6	A	508	FUC	O5-C1	-2.35	1.39	1.43
3	B	501	NAG	O5-C5	-2.31	1.38	1.43
7	B	509	GAL	O3-C3	-2.30	1.37	1.43
5	A	504	MAN	O2-C2	-2.24	1.38	1.43
3	B	501	NAG	C2-N2	-2.01	1.42	1.46
6	B	508	FUC	O2-C2	2.16	1.48	1.43
5	C	307	MAN	C1-C2	2.21	1.57	1.52
7	A	509	GAL	C2-C3	2.27	1.55	1.52
3	A	502	NAG	C8-C7	2.32	1.55	1.50
7	A	509	GAL	C1-C2	2.38	1.57	1.52
3	B	501	NAG	C1-C2	2.50	1.55	1.52
7	A	509	GAL	O5-C1	2.61	1.48	1.43
3	C	303	NAG	C1-C2	2.88	1.56	1.52
7	A	509	GAL	O2-C2	4.33	1.53	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	308	MAN	C1-C2-C3	-8.38	99.62	109.54
5	C	307	MAN	C1-O5-C5	-7.02	103.34	112.25
5	C	308	MAN	C1-O5-C5	-6.79	103.63	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	307	MAN	C1-C2-C3	-5.54	102.98	109.54
6	B	508	FUC	C1-C2-C3	-5.44	103.10	109.54
6	A	508	FUC	O2-C2-C3	-5.36	99.34	110.12
5	A	506	MAN	O4-C4-C3	-4.09	101.13	110.34
5	C	307	MAN	O2-C2-C3	-4.03	102.01	110.12
7	A	509	GAL	C1-C2-C3	-4.02	104.78	109.54
5	C	308	MAN	O3-C3-C2	-4.00	102.77	110.00
3	C	303	NAG	O4-C4-C3	-3.82	101.73	110.34
5	A	506	MAN	O5-C1-C2	-3.82	104.66	110.86
5	A	504	MAN	O2-C2-C3	-3.72	102.63	110.12
5	C	307	MAN	O6-C6-C5	-3.64	99.31	111.33
5	B	504	MAN	O2-C2-C1	-3.53	102.14	109.21
3	C	303	NAG	C3-C2-N2	-3.50	102.17	110.56
3	A	501	NAG	O6-C6-C5	-3.37	100.21	111.33
7	A	509	GAL	O3-C3-C4	-3.17	103.20	110.34
3	A	501	NAG	O7-C7-N2	-3.16	115.41	121.86
5	A	506	MAN	O2-C2-C1	-3.05	103.10	109.21
3	A	505	NAG	O4-C4-C3	-3.04	103.49	110.34
3	C	301	NAG	O7-C7-C8	-3.03	116.51	122.06
5	B	504	MAN	O6-C6-C5	-2.90	101.74	111.33
3	C	302	NAG	C3-C2-N2	-2.89	103.63	110.56
5	B	506	MAN	C3-C4-C5	-2.83	105.26	110.20
5	B	506	MAN	C2-C3-C4	-2.76	106.36	111.04
5	C	307	MAN	C2-C3-C4	-2.74	106.38	111.04
5	B	506	MAN	O4-C4-C3	-2.72	104.21	110.34
3	B	502	NAG	C6-C5-C4	-2.72	106.31	113.02
3	C	302	NAG	O7-C7-C8	-2.69	117.12	122.06
6	A	508	FUC	O4-C4-C3	-2.66	104.34	110.34
6	A	508	FUC	O5-C1-C2	-2.64	106.57	110.86
3	B	502	NAG	C1-O5-C5	-2.52	109.05	112.25
3	A	502	NAG	O6-C6-C5	-2.49	103.11	111.33
3	B	502	NAG	O4-C4-C5	-2.42	102.81	109.24
3	C	304	NAG	C2-N2-C7	-2.38	119.98	123.04
5	B	506	MAN	O5-C1-C2	-2.38	107.00	110.86
3	B	505	NAG	C2-N2-C7	-2.34	120.03	123.04
5	C	307	MAN	O4-C4-C3	-2.31	105.14	110.34
3	A	502	NAG	O7-C7-C8	-2.29	117.87	122.06
3	B	505	NAG	O4-C4-C3	-2.27	105.22	110.34
7	B	509	GAL	C3-C4-C5	-2.20	106.36	110.20
3	B	507	NAG	O7-C7-C8	-2.16	118.10	122.06
5	B	504	MAN	C6-C5-C4	-2.15	107.70	113.02
3	A	507	NAG	O7-C7-C8	-2.14	118.13	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	O4-C4-C5	-2.11	103.64	109.24
5	C	306	MAN	O2-C2-C3	-2.11	105.88	110.12
5	A	504	MAN	C6-C5-C4	-2.05	107.95	113.02
7	A	509	GAL	O3-C3-C2	-2.02	106.34	110.00
6	B	508	FUC	C6-C5-C4	-2.01	109.12	113.08
5	C	308	MAN	O4-C4-C3	2.02	114.89	110.34
7	A	509	GAL	O5-C5-C6	2.05	111.80	107.35
5	A	504	MAN	C1-O5-C5	2.06	114.87	112.25
5	C	306	MAN	C1-C2-C3	2.11	112.04	109.54
6	A	508	FUC	C1-C2-C3	2.12	112.04	109.54
5	A	506	MAN	C1-C2-C3	2.13	112.06	109.54
6	A	508	FUC	O2-C2-C1	2.23	113.67	109.21
3	A	501	NAG	O3-C3-C4	2.28	115.47	110.34
6	B	508	FUC	C1-O5-C5	2.47	116.20	112.38
5	C	306	MAN	C1-O5-C5	2.63	115.58	112.25
3	B	502	NAG	O5-C5-C6	2.64	113.06	107.35
6	A	508	FUC	O5-C5-C4	2.64	114.11	109.53
3	A	507	NAG	C1-O5-C5	2.66	115.63	112.25
5	B	506	MAN	C1-O5-C5	2.69	115.66	112.25
3	C	302	NAG	C4-C3-C2	2.76	115.52	111.23
3	B	507	NAG	C4-C3-C2	2.76	115.53	111.23
3	B	507	NAG	C2-N2-C7	2.77	126.60	123.04
3	C	301	NAG	C1-O5-C5	2.78	115.77	112.25
3	C	302	NAG	C3-C4-C5	2.78	115.05	110.20
7	B	509	GAL	C2-C3-C4	2.86	115.89	111.04
3	C	302	NAG	C2-N2-C7	2.96	126.84	123.04
5	C	306	MAN	O3-C3-C2	2.98	115.39	110.00
5	A	504	MAN	C1-C2-C3	2.99	113.08	109.54
3	A	501	NAG	C8-C7-N2	3.11	122.07	116.11
5	C	308	MAN	O5-C5-C6	3.14	114.15	107.35
5	B	504	MAN	C1-C2-C3	3.18	113.30	109.54
7	A	509	GAL	C1-O5-C5	3.32	116.47	112.25
3	B	507	NAG	C3-C4-C5	3.37	116.07	110.20
7	B	509	GAL	O2-C2-C1	3.49	116.20	109.21
5	C	307	MAN	C3-C4-C5	3.58	116.43	110.20
5	C	308	MAN	O5-C1-C2	3.80	117.02	110.86
5	B	504	MAN	C1-O5-C5	4.34	117.76	112.25
7	A	509	GAL	C2-C3-C4	5.31	120.05	111.04
3	A	501	NAG	C1-O5-C5	5.61	119.37	112.25
6	B	508	FUC	O2-C2-C1	6.09	121.41	109.21
7	A	509	GAL	O2-C2-C1	6.15	121.54	109.21
5	C	307	MAN	O5-C1-C2	6.35	121.15	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	509	GAL	C1-O5-C5	7.88	122.25	112.25
3	C	302	NAG	C1-O5-C5	7.89	122.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	509	GAL	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 6 are monoatomic - leaving 37 for Mogul analysis.

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	501	1,3,6	14,14,15	1.07	0	15,19,21	2.35	5 (33%)
3	NAG	A	502	3,4	14,14,15	1.37	2 (14%)	15,19,21	1.44	3 (20%)
4	BMA	A	503	3,5	11,11,12	0.84	0	14,15,17	2.23	7 (50%)
5	MAN	A	504	3,4	11,11,12	0.84	1 (9%)	14,15,17	1.76	4 (28%)
3	NAG	A	505	5,7	14,14,15	0.86	1 (7%)	15,19,21	1.07	1 (6%)
5	MAN	A	506	3,4	11,11,12	0.87	0	14,15,17	2.05	4 (28%)
3	NAG	A	507	5	14,14,15	0.74	0	15,19,21	1.26	2 (13%)
6	FUC	A	508	3	10,10,11	1.09	1 (10%)	14,14,16	2.18	6 (42%)
7	GAL	A	509	3	11,11,12	2.23	5 (45%)	14,15,17	2.94	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ACT	A	513	8	1,3,3	2.50	1 (100%)	0,3,3	0.00	-
9	ACT	A	514	-	1,3,3	3.64	1 (100%)	0,3,3	0.00	-
9	ACT	A	515	8	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
9	ACT	A	516	-	1,3,3	0.72	0	0,3,3	0.00	-
9	ACT	A	517	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
9	ACT	A	518	-	1,3,3	1.73	0	0,3,3	0.00	-
10	GOL	A	519	-	5,5,5	0.33	0	5,5,5	0.53	0
3	NAG	B	501	1,3,6	14,14,15	1.34	4 (28%)	15,19,21	1.06	0
3	NAG	B	502	3,4	14,14,15	0.94	0	15,19,21	1.46	4 (26%)
4	BMA	B	503	3,5	11,11,12	0.76	0	14,15,17	1.59	4 (28%)
5	MAN	B	504	3,4	11,11,12	1.07	0	14,15,17	2.15	5 (35%)
3	NAG	B	505	5,7	14,14,15	0.91	0	15,19,21	1.19	2 (13%)
5	MAN	B	506	3,4	11,11,12	1.10	0	14,15,17	1.73	5 (35%)
3	NAG	B	507	5	14,14,15	0.65	0	15,19,21	1.61	4 (26%)
6	FUC	B	508	3	10,10,11	0.98	1 (10%)	14,14,16	2.48	4 (28%)
7	GAL	B	509	3	11,11,12	1.26	1 (9%)	14,15,17	2.57	4 (28%)
9	ACT	B	512	8	1,3,3	1.51	0	0,3,3	0.00	-
10	GOL	B	513	-	5,5,5	0.33	0	5,5,5	0.59	0
3	NAG	C	301	3,2	14,14,15	0.77	0	15,19,21	1.26	2 (13%)
3	NAG	C	302	3	14,14,15	0.64	0	15,19,21	2.74	6 (40%)
3	NAG	C	303	3,2	14,14,15	0.91	1 (7%)	15,19,21	1.65	2 (13%)
3	NAG	C	304	3,4	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
4	BMA	C	305	3,5	11,11,12	1.10	1 (9%)	14,15,17	1.75	4 (28%)
5	MAN	C	306	5,4	11,11,12	1.14	0	14,15,17	1.57	4 (28%)
5	MAN	C	307	5	11,11,12	1.39	2 (18%)	14,15,17	3.60	8 (57%)
5	MAN	C	308	5	11,11,12	0.98	0	14,15,17	3.45	6 (42%)
9	ACT	C	310	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
9	ACT	C	311	-	1,3,3	1.35	0	0,3,3	0.00	-

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	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	503	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	5,7	-	0/6/23/26	0/1/1/1
5	MAN	A	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	507	5	-	0/6/23/26	0/1/1/1
6	FUC	A	508	3	-	0/0/17/20	0/1/1/1
7	GAL	A	509	3	-	0/2/19/22	0/1/1/1
9	ACT	A	513	8	-	0/0/0/0	0/0/0/0
9	ACT	A	514	-	-	0/0/0/0	0/0/0/0
9	ACT	A	515	8	-	0/0/0/0	0/0/0/0
9	ACT	A	516	-	-	0/0/0/0	0/0/0/0
9	ACT	A	517	-	-	0/0/0/0	0/0/0/0
9	ACT	A	518	-	-	0/0/0/0	0/0/0/0
10	GOL	A	519	-	-	0/4/4/4	0/0/0/0
3	NAG	B	501	1,3,6	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	503	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	505	5,7	-	0/6/23/26	0/1/1/1
5	MAN	B	506	3,4	-	0/2/19/22	0/1/1/1
3	NAG	B	507	5	-	0/6/23/26	0/1/1/1
6	FUC	B	508	3	-	0/0/17/20	0/1/1/1
7	GAL	B	509	3	-	0/2/19/22	0/1/1/1
9	ACT	B	512	8	-	0/0/0/0	0/0/0/0
10	GOL	B	513	-	-	0/4/4/4	0/0/0/0
3	NAG	C	301	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	302	3	-	0/6/23/26	0/1/1/1
3	NAG	C	303	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	304	3,4	-	0/6/23/26	0/1/1/1
4	BMA	C	305	3,5	-	0/2/19/22	0/1/1/1
5	MAN	C	306	5,4	-	0/2/19/22	0/1/1/1
5	MAN	C	307	5	-	0/2/19/22	0/1/1/1
5	MAN	C	308	5	-	0/2/19/22	0/1/1/1
9	ACT	C	310	-	-	0/0/0/0	0/0/0/0
9	ACT	C	311	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	O5-C1	-4.10	1.36	1.43
7	A	509	GAL	O3-C3	-4.01	1.33	1.43
5	C	307	MAN	O5-C1	-3.19	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	NAG	O5-C1	-2.62	1.39	1.43
3	A	505	NAG	O5-C5	-2.38	1.38	1.43
6	A	508	FUC	O5-C1	-2.35	1.39	1.43
3	B	501	NAG	O5-C5	-2.31	1.38	1.43
7	B	509	GAL	O3-C3	-2.30	1.37	1.43
5	A	504	MAN	O2-C2	-2.24	1.38	1.43
3	B	501	NAG	C2-N2	-2.01	1.42	1.46
6	B	508	FUC	O2-C2	2.16	1.48	1.43
5	C	307	MAN	C1-C2	2.21	1.57	1.52
7	A	509	GAL	C2-C3	2.27	1.55	1.52
3	A	502	NAG	C8-C7	2.32	1.55	1.50
9	A	517	ACT	CH3-C	2.37	1.52	1.48
7	A	509	GAL	C1-C2	2.38	1.57	1.52
4	C	305	BMA	C4-C5	2.42	1.58	1.53
9	A	513	ACT	CH3-C	2.50	1.52	1.48
3	B	501	NAG	C1-C2	2.50	1.55	1.52
7	A	509	GAL	O5-C1	2.61	1.48	1.43
9	C	310	ACT	CH3-C	2.61	1.52	1.48
3	C	303	NAG	C1-C2	2.88	1.56	1.52
9	A	515	ACT	CH3-C	3.53	1.53	1.48
9	A	514	ACT	CH3-C	3.64	1.53	1.48
7	A	509	GAL	O2-C2	4.33	1.53	1.43

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	308	MAN	C1-C2-C3	-8.38	99.62	109.54
5	C	307	MAN	C1-O5-C5	-7.02	103.34	112.25
5	C	308	MAN	C1-O5-C5	-6.79	103.63	112.25
5	C	307	MAN	C1-C2-C3	-5.54	102.98	109.54
6	B	508	FUC	C1-C2-C3	-5.44	103.10	109.54
6	A	508	FUC	O2-C2-C3	-5.36	99.34	110.12
4	A	503	BMA	O3-C3-C2	-4.10	102.60	110.00
5	A	506	MAN	O4-C4-C3	-4.09	101.13	110.34
5	C	307	MAN	O2-C2-C3	-4.03	102.01	110.12
7	A	509	GAL	C1-C2-C3	-4.02	104.78	109.54
5	C	308	MAN	O3-C3-C2	-4.00	102.77	110.00
3	C	303	NAG	O4-C4-C3	-3.82	101.73	110.34
5	A	506	MAN	O5-C1-C2	-3.82	104.66	110.86
5	A	504	MAN	O2-C2-C3	-3.72	102.63	110.12
5	C	307	MAN	O6-C6-C5	-3.64	99.31	111.33
5	B	504	MAN	O2-C2-C1	-3.53	102.14	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	NAG	C3-C2-N2	-3.50	102.17	110.56
4	B	503	BMA	O4-C4-C3	-3.48	102.51	110.34
3	A	501	NAG	O6-C6-C5	-3.37	100.21	111.33
4	A	503	BMA	O4-C4-C3	-3.36	102.78	110.34
7	A	509	GAL	O3-C3-C4	-3.17	103.20	110.34
3	A	501	NAG	O7-C7-N2	-3.16	115.41	121.86
5	A	506	MAN	O2-C2-C1	-3.05	103.10	109.21
3	A	505	NAG	O4-C4-C3	-3.04	103.49	110.34
3	C	301	NAG	O7-C7-C8	-3.03	116.51	122.06
5	B	504	MAN	O6-C6-C5	-2.90	101.74	111.33
3	C	302	NAG	C3-C2-N2	-2.89	103.63	110.56
5	B	506	MAN	C3-C4-C5	-2.83	105.26	110.20
4	B	503	BMA	C1-O5-C5	-2.82	108.67	112.25
5	B	506	MAN	C2-C3-C4	-2.76	106.36	111.04
5	C	307	MAN	C2-C3-C4	-2.74	106.38	111.04
5	B	506	MAN	O4-C4-C3	-2.72	104.21	110.34
3	B	502	NAG	C6-C5-C4	-2.72	106.31	113.02
3	C	302	NAG	O7-C7-C8	-2.69	117.12	122.06
6	A	508	FUC	O4-C4-C3	-2.66	104.34	110.34
6	A	508	FUC	O5-C1-C2	-2.64	106.57	110.86
4	A	503	BMA	C1-C2-C3	-2.64	106.42	109.54
3	B	502	NAG	C1-O5-C5	-2.52	109.05	112.25
4	A	503	BMA	O2-C2-C1	-2.49	104.22	109.21
3	A	502	NAG	O6-C6-C5	-2.49	103.11	111.33
4	A	503	BMA	C3-C4-C5	-2.43	105.96	110.20
3	B	502	NAG	O4-C4-C5	-2.42	102.81	109.24
4	A	503	BMA	C1-O5-C5	-2.39	109.21	112.25
3	C	304	NAG	C2-N2-C7	-2.38	119.98	123.04
5	B	506	MAN	O5-C1-C2	-2.38	107.00	110.86
3	B	505	NAG	C2-N2-C7	-2.34	120.03	123.04
5	C	307	MAN	O4-C4-C3	-2.31	105.14	110.34
3	A	502	NAG	O7-C7-C8	-2.29	117.87	122.06
3	B	505	NAG	O4-C4-C3	-2.27	105.22	110.34
4	A	503	BMA	O3-C3-C4	-2.26	105.26	110.34
4	B	503	BMA	C6-C5-C4	-2.22	107.55	113.02
4	B	503	BMA	O2-C2-C1	-2.21	104.77	109.21
7	B	509	GAL	C3-C4-C5	-2.20	106.36	110.20
3	B	507	NAG	O7-C7-C8	-2.16	118.10	122.06
5	B	504	MAN	C6-C5-C4	-2.15	107.70	113.02
3	A	507	NAG	O7-C7-C8	-2.14	118.13	122.06
3	A	502	NAG	O4-C4-C5	-2.11	103.64	109.24
5	C	306	MAN	O2-C2-C3	-2.11	105.88	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	MAN	C6-C5-C4	-2.05	107.95	113.02
7	A	509	GAL	O3-C3-C2	-2.02	106.34	110.00
6	B	508	FUC	C6-C5-C4	-2.01	109.12	113.08
5	C	308	MAN	O4-C4-C3	2.02	114.89	110.34
7	A	509	GAL	O5-C5-C6	2.05	111.80	107.35
5	A	504	MAN	C1-O5-C5	2.06	114.87	112.25
4	C	305	BMA	C6-C5-C4	2.11	118.21	113.02
5	C	306	MAN	C1-C2-C3	2.11	112.04	109.54
6	A	508	FUC	C1-C2-C3	2.12	112.04	109.54
5	A	506	MAN	C1-C2-C3	2.13	112.06	109.54
6	A	508	FUC	O2-C2-C1	2.23	113.67	109.21
3	A	501	NAG	O3-C3-C4	2.28	115.47	110.34
4	C	305	BMA	O4-C4-C5	2.41	115.64	109.24
6	B	508	FUC	C1-O5-C5	2.47	116.20	112.38
5	C	306	MAN	C1-O5-C5	2.63	115.58	112.25
3	B	502	NAG	O5-C5-C6	2.64	113.06	107.35
6	A	508	FUC	O5-C5-C4	2.64	114.11	109.53
3	A	507	NAG	C1-O5-C5	2.66	115.63	112.25
5	B	506	MAN	C1-O5-C5	2.69	115.66	112.25
3	C	302	NAG	C4-C3-C2	2.76	115.52	111.23
3	B	507	NAG	C4-C3-C2	2.76	115.53	111.23
3	B	507	NAG	C2-N2-C7	2.77	126.60	123.04
3	C	301	NAG	C1-O5-C5	2.78	115.77	112.25
3	C	302	NAG	C3-C4-C5	2.78	115.05	110.20
4	C	305	BMA	O6-C6-C5	2.82	120.64	111.33
7	B	509	GAL	C2-C3-C4	2.86	115.89	111.04
3	C	302	NAG	C2-N2-C7	2.96	126.84	123.04
5	C	306	MAN	O3-C3-C2	2.98	115.39	110.00
5	A	504	MAN	C1-C2-C3	2.99	113.08	109.54
3	A	501	NAG	C8-C7-N2	3.11	122.07	116.11
5	C	308	MAN	O5-C5-C6	3.14	114.15	107.35
5	B	504	MAN	C1-C2-C3	3.18	113.30	109.54
7	A	509	GAL	C1-O5-C5	3.32	116.47	112.25
3	B	507	NAG	C3-C4-C5	3.37	116.07	110.20
7	B	509	GAL	O2-C2-C1	3.49	116.20	109.21
5	C	307	MAN	C3-C4-C5	3.58	116.43	110.20
5	C	308	MAN	O5-C1-C2	3.80	117.02	110.86
4	C	305	BMA	O5-C5-C6	3.97	115.94	107.35
5	B	504	MAN	C1-O5-C5	4.34	117.76	112.25
7	A	509	GAL	C2-C3-C4	5.31	120.05	111.04
3	A	501	NAG	C1-O5-C5	5.61	119.37	112.25
6	B	508	FUC	O2-C2-C1	6.09	121.41	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	509	GAL	O2-C2-C1	6.15	121.54	109.21
5	C	307	MAN	O5-C1-C2	6.35	121.15	110.86
7	B	509	GAL	C1-O5-C5	7.88	122.25	112.25
3	C	302	NAG	C1-O5-C5	7.89	122.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	514	ACT	1	0
7	B	509	GAL	1	0
10	B	513	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	215/224 (95%)	-0.20	2 (0%) 85 83	26, 34, 51, 75	0
1	B	209/224 (93%)	-0.32	2 (0%) 84 82	27, 38, 55, 87	0
2	C	259/280 (92%)	0.22	25 (9%) 10 7	28, 40, 90, 119	0
All	All	683/728 (93%)	-0.08	29 (4%) 40 34	26, 37, 71, 119	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	GLY	7.2
2	C	64	GLN	7.1
2	C	51	SER	6.9
2	C	89	LEU	6.1
1	B	235	LEU	5.3
2	C	65	THR	5.2
2	C	23	VAL	4.8
2	C	222	GLY	4.6
2	C	63	ILE	4.6
2	C	221	PRO	4.5
2	C	45	VAL	4.5
2	C	53	SER	4.3
2	C	67	THR	4.2
2	C	87	ARG	4.1
2	C	90	SER	4.1
2	C	52	SER	3.6
2	C	223	LEU	3.4
2	C	219	GLN	3.1
2	C	91	GLY	3.1
2	C	88	GLY	3.0
2	C	66	SER	3.0
2	C	54	THR	2.7
2	C	49	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	22	ALA	2.6
1	B	389[A]	ASN	2.5
1	A	232	PRO	2.5
1	A	314	LEU	2.4
2	C	149	TRP	2.1
2	C	44	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	GAL	A	509	11/12	0.84	0.25	8.65	37,49,58,64	0
7	GAL	B	509	11/12	0.91	0.22	5.41	41,51,56,58	0
5	MAN	C	308	11/12	0.89	0.13	1.63	49,53,58,59	0
3	NAG	A	501	14/15	0.96	0.07	-0.52	31,35,40,42	0
3	NAG	A	502	14/15	0.97	0.07	-0.57	30,34,39,40	0
3	NAG	C	301	14/15	0.95	0.09	-0.88	44,55,68,71	0
3	NAG	B	502	14/15	0.97	0.07	-0.92	33,37,41,41	0
3	NAG	A	505	14/15	0.96	0.06	-1.09	37,44,48,50	0
3	NAG	B	501	14/15	0.98	0.06	-1.11	32,34,41,46	0
6	FUC	B	508	10/11	0.89	0.14	-	54,62,69,77	0
5	MAN	A	506	11/12	0.94	0.11	-	36,53,65,67	0
3	NAG	C	302	14/15	0.79	0.35	-	83,92,100,101	0
3	NAG	B	507	14/15	0.72	0.30	-	92,102,114,115	0
3	NAG	C	303	14/15	0.87	0.19	-	53,64,72,78	0
5	MAN	B	504	11/12	0.96	0.07	-	39,44,51,52	0
5	MAN	C	307	11/12	0.86	0.17	-	46,52,56,57	0
6	FUC	A	508	10/11	0.95	0.09	-	48,51,56,59	0
5	MAN	B	506	11/12	0.91	0.12	-	52,61,82,84	0
5	MAN	C	306	11/12	0.92	0.17	-	52,55,60,65	0
3	NAG	B	505	14/15	0.92	0.08	-	42,48,51,53	0
3	NAG	C	304	14/15	0.81	0.27	-	59,66,71,72	0
5	MAN	A	504	11/12	0.97	0.05	-	38,39,45,47	0
3	NAG	A	507	14/15	0.83	0.24	-	78,88,102,107	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	GAL	A	509	11/12	0.84	0.25	8.65	37,49,58,64	0
10	GOL	B	513	6/6	0.87	0.25	8.21	63,66,70,79	0
7	GAL	B	509	11/12	0.91	0.22	5.41	41,51,56,58	0
9	ACT	A	517	4/4	0.80	0.17	3.46	67,69,70,75	0
9	ACT	A	516	4/4	0.94	0.17	2.95	47,56,57,61	0
9	ACT	B	512	4/4	0.94	0.10	2.06	39,39,45,48	0
5	MAN	C	308	11/12	0.89	0.13	1.63	49,53,58,59	0
10	GOL	A	519	6/6	0.90	0.13	1.27	62,67,71,71	0
9	ACT	A	513	4/4	0.97	0.14	0.16	27,33,33,40	0
8	ZN	A	510	1/1	0.99	0.09	-0.36	34,34,34,34	0
9	ACT	A	515	4/4	0.96	0.10	-0.42	29,40,41,42	0
3	NAG	A	501	14/15	0.96	0.07	-0.52	31,35,40,42	0
3	NAG	A	502	14/15	0.97	0.07	-0.57	30,34,39,40	0
3	NAG	C	301	14/15	0.95	0.09	-0.88	44,55,68,71	0
3	NAG	B	502	14/15	0.97	0.07	-0.92	33,37,41,41	0
3	NAG	A	505	14/15	0.96	0.06	-1.09	37,44,48,50	0
3	NAG	B	501	14/15	0.98	0.06	-1.11	32,34,41,46	0
8	ZN	A	511	1/1	0.98	0.04	-4.84	42,42,42,42	0
3	NAG	B	507	14/15	0.72	0.30	-	92,102,114,115	0
5	MAN	C	307	11/12	0.86	0.17	-	46,52,56,57	0
5	MAN	B	506	11/12	0.91	0.12	-	52,61,82,84	0
9	ACT	C	311	4/4	0.93	0.10	-	45,46,52,55	4
3	NAG	B	505	14/15	0.92	0.08	-	42,48,51,53	0
6	FUC	B	508	10/11	0.89	0.14	-	54,62,69,77	0
4	BMA	A	503	11/12	0.97	0.07	-	30,33,36,37	0
8	ZN	B	511	1/1	1.00	0.10	-	30,30,30,30	0
5	MAN	A	506	11/12	0.94	0.11	-	36,53,65,67	0
4	BMA	C	305	11/12	0.78	0.26	-	48,58,67,67	0
8	ZN	C	309	1/1	0.96	0.06	-	54,54,54,54	1
3	NAG	C	303	14/15	0.87	0.19	-	53,64,72,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MAN	B	504	11/12	0.96	0.07	-	39,44,51,52	0
8	ZN	B	510	1/1	1.00	0.07	-	50,50,50,50	0
9	ACT	C	310	4/4	0.66	0.24	-	67,73,74,75	0
8	ZN	A	512	1/1	0.97	0.03	-	62,62,62,62	0
6	FUC	A	508	10/11	0.95	0.09	-	48,51,56,59	0
3	NAG	C	302	14/15	0.79	0.35	-	83,92,100,101	0
4	BMA	B	503	11/12	0.95	0.06	-	32,41,46,51	0
5	MAN	C	306	11/12	0.92	0.17	-	52,55,60,65	0
9	ACT	A	518	4/4	0.86	0.28	-	60,65,66,71	0
3	NAG	C	304	14/15	0.81	0.27	-	59,66,71,72	0
5	MAN	A	504	11/12	0.97	0.05	-	38,39,45,47	0
3	NAG	A	507	14/15	0.83	0.24	-	78,88,102,107	0
9	ACT	A	514	4/4	0.82	0.26	-	49,59,61,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.