



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2017 – 06:09 PM EST

PDB ID : 5HYI
Title : Glycosylated, disulfide-linked Hole-Hole Fc fragment
Authors : Kuglstatter, A.; Stihle, M.; Benz, J.
Deposited on : unknown
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

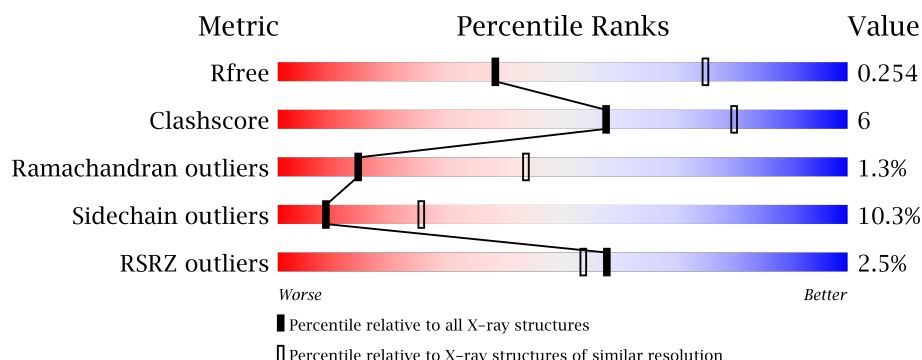
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	227	<div> <div>74%</div> <div>18%</div> <div>8%</div> </div>
1	B	227	<div> <div>3%</div> <div>66%</div> <div>23%</div> <div>8%</div> </div>
1	C	227	<div> <div>6%</div> <div>67%</div> <div>23%</div> <div>8%</div> </div>
1	D	227	<div> <div>70%</div> <div>20%</div> <div>8%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7251 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.

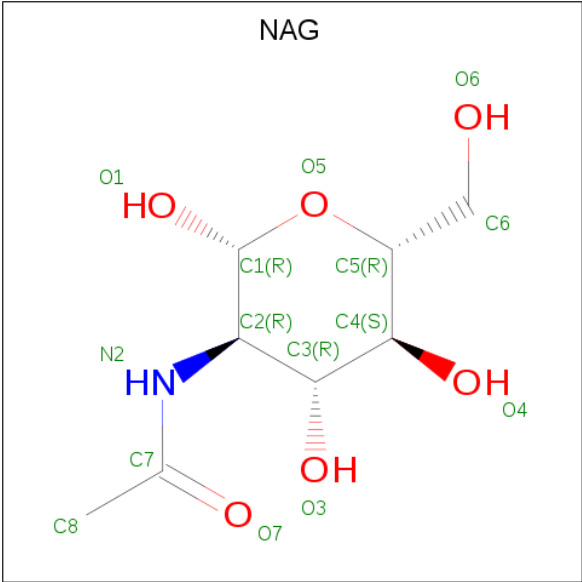
- Molecule 1 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1656	1050	281	318	7			
1	B	209	Total	C	N	O	S	0	0	0
			1653	1047	281	318	7			
1	C	208	Total	C	N	O	S	0	0	0
			1649	1045	280	317	7			
1	D	209	Total	C	N	O	S	0	0	0
			1653	1047	281	318	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	CYS	TYR	engineered mutation	UNP P01857
A	366	SER	THR	engineered mutation	UNP P01857
A	368	ALA	LEU	engineered mutation	UNP P01857
A	407	VAL	TYR	engineered mutation	UNP P01857
B	349	CYS	TYR	engineered mutation	UNP P01857
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857
C	349	CYS	TYR	engineered mutation	UNP P01857
C	366	SER	THR	engineered mutation	UNP P01857
C	368	ALA	LEU	engineered mutation	UNP P01857
C	407	VAL	TYR	engineered mutation	UNP P01857
D	349	CYS	TYR	engineered mutation	UNP P01857
D	366	SER	THR	engineered mutation	UNP P01857
D	368	ALA	LEU	engineered mutation	UNP P01857
D	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



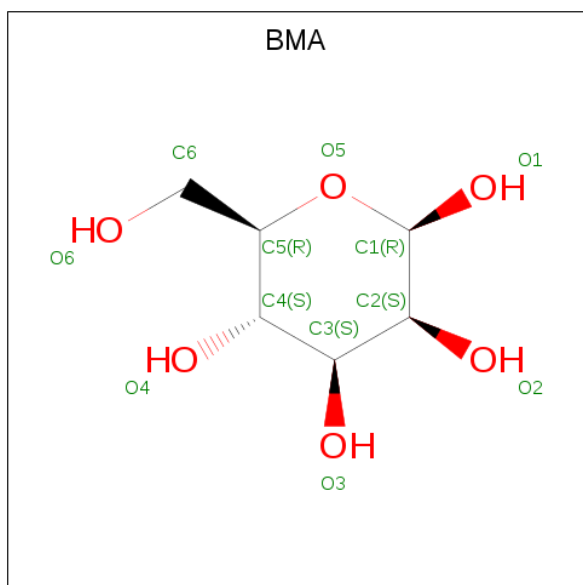
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



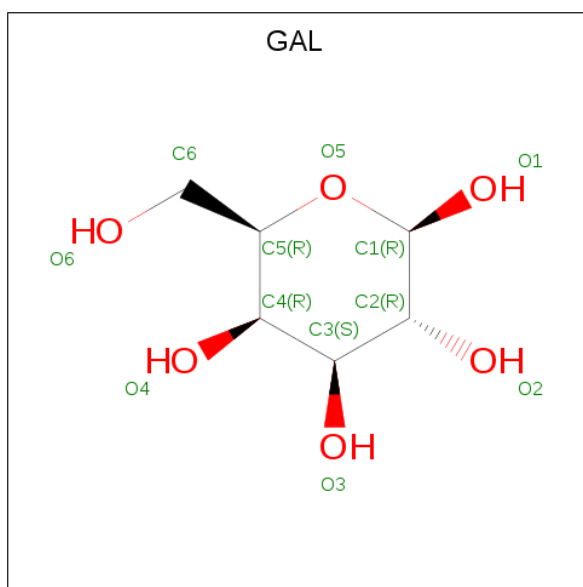
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

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



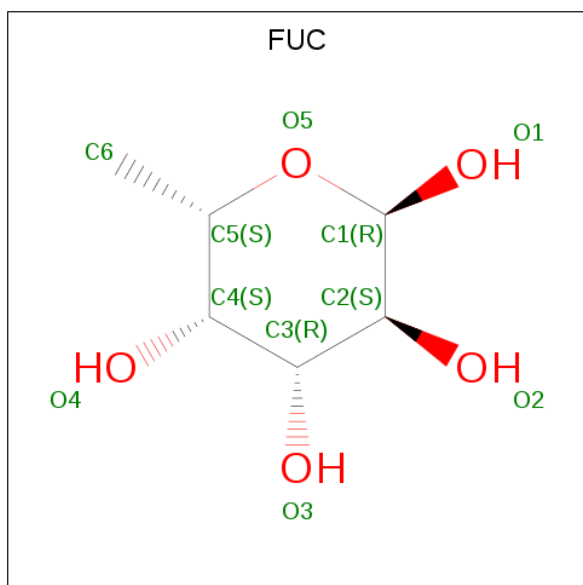
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

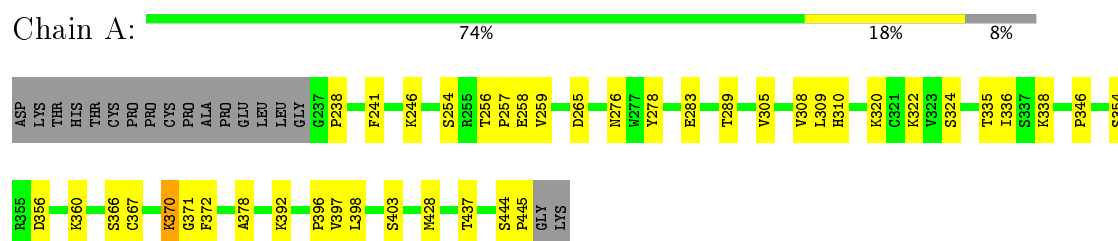
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total	O	0	0
			66	66		
7	B	29	Total	O	0	0
			29	29		
7	C	33	Total	O	0	0
			33	33		
7	D	72	Total	O	0	0
			72	72		

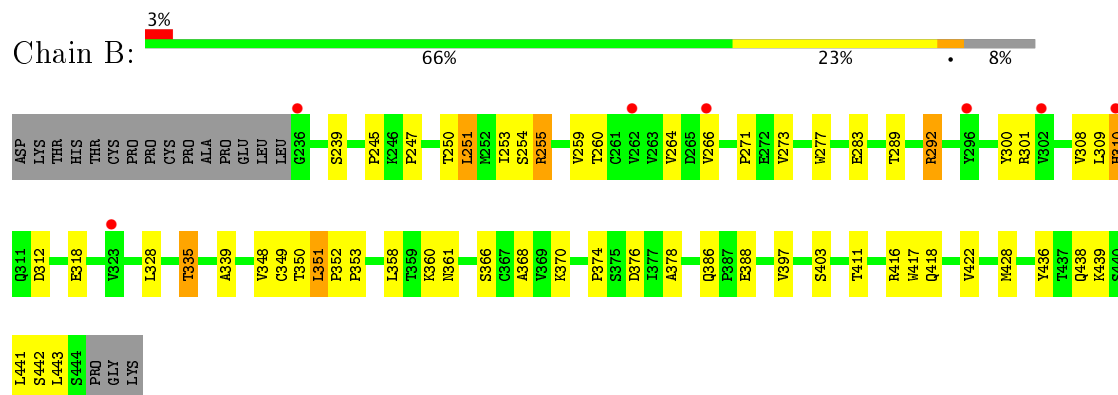
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

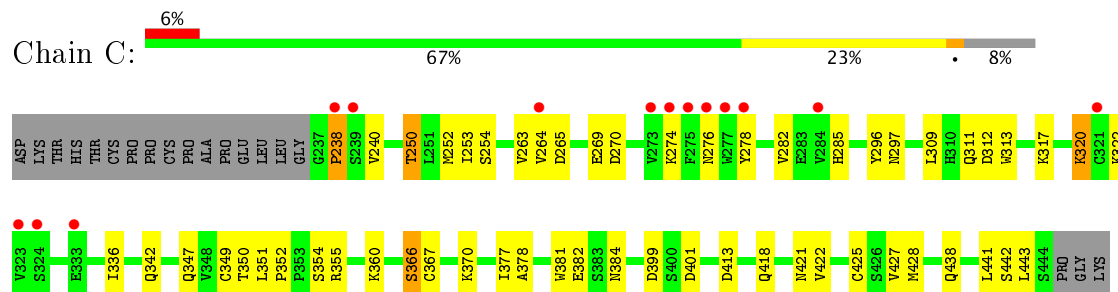
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

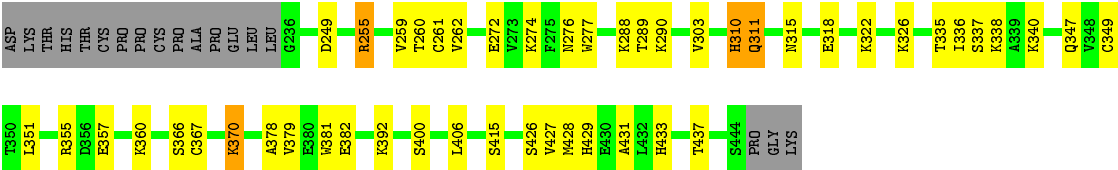


- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.28Å 105.66Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.90 49.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.15-2.90) 99.5 (49.17-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.175 , 0.235 0.197 , 0.254	Depositor DCC
R_{free} test set	1677 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.01% 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: MAN, GAL, BMA, NAG, FUC

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	0.58	0/1701	0.79	0/2318
1	B	0.52	0/1697	0.75	0/2311
1	C	0.53	0/1693	0.72	0/2306
1	D	0.56	0/1697	0.78	0/2311
All	All	0.55	0/6788	0.76	0/9246

There are no bond length outliers.

There are no bond angle outliers.

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	1656	0	1624	14	0
1	B	1653	0	1620	25	0
1	C	1649	0	1617	24	0
1	D	1653	0	1620	21	0
2	A	56	0	48	1	0
2	B	56	0	48	0	0
2	C	56	0	48	0	0
2	D	56	0	48	1	0
3	A	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	8	0	0
3	C	11	0	8	0	0
3	D	11	0	8	1	0
4	A	22	0	18	0	0
4	B	22	0	18	0	0
4	C	22	0	18	0	0
4	D	22	0	18	1	0
5	A	11	0	10	0	0
5	B	11	0	10	0	0
5	C	11	0	10	0	0
5	D	11	0	10	0	0
6	A	10	0	10	0	0
6	B	10	0	10	0	0
6	C	10	0	10	1	0
6	D	10	0	10	0	0
7	A	66	0	0	0	0
7	B	29	0	0	1	0
7	C	33	0	0	1	0
7	D	72	0	0	1	0
All	All	7251	0	6857	78	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 (78) 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:B:422:VAL:HG22	1:B:442:SER:HB3	1.63	0.79
1:B:386:GLN:HG2	1:D:355:ARG:HG2	1.70	0.74
1:D:259:VAL:HG13	1:D:336:ILE:HD11	1.75	0.69
1:C:278:TYR:HB2	1:C:320:LYS:HB2	1.76	0.67
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.79	0.64
1:C:347:GLN:HB3	1:D:351:LEU:HD22	1.79	0.64
1:A:259:VAL:HG13	1:A:336:ILE:HD11	1.79	0.64
1:C:367:CYS:HB2	1:C:381:TRP:CZ2	2.33	0.63
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.83	0.60
1:D:378:ALA:HB3	1:D:428:MET:HB2	1.86	0.57
1:C:238:PRO:HA	1:C:265:ASP:HB2	1.87	0.57
1:B:348:VAL:HB	1:B:439:LYS:HG3	1.85	0.56
1:B:308:VAL:HA	7:B:615:HOH:O	2.05	0.56
1:D:249:ASP:HA	1:D:255:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:HB3	1:A:428:MET:HB2	1.88	0.55
1:C:425:CYS:O	1:C:438:GLN:HA	2.06	0.55
1:D:274:LYS:NZ	1:D:276:ASN:HD21	2.05	0.55
1:D:429:HIS:HD2	1:D:431:ALA:H	1.55	0.55
1:C:378:ALA:HB3	1:C:428:MET:HB2	1.89	0.55
1:C:350:THR:HB	1:C:441:LEU:HD22	1.88	0.54
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.88	0.54
1:C:418:GLN:HA	1:C:443:LEU:HD22	1.89	0.54
1:D:276:ASN:HB2	1:D:322:LYS:HB3	1.89	0.53
1:C:355:ARG:HH22	1:D:433:HIS:HB2	1.73	0.53
1:C:250:THR:HG21	1:C:313:TRP:CD1	2.44	0.53
1:B:247:PRO:O	1:B:251:LEU:HD22	2.08	0.52
1:C:276:ASN:HB2	1:C:322:LYS:HB3	1.91	0.52
1:D:351:LEU:HB2	1:D:366:SER:HB2	1.89	0.52
1:D:262:VAL:HG22	1:D:303:VAL:HG22	1.91	0.51
1:B:352:PRO:HB2	1:B:353:PRO:CD	2.42	0.50
1:A:238:PRO:HA	1:A:265:ASP:HB2	1.95	0.49
1:B:339:ALA:HB3	1:B:374:PRO:HB3	1.94	0.49
1:C:366:SER:HB3	1:D:370:LYS:HD3	1.95	0.49
1:A:278:TYR:CE2	1:A:283:GLU:HB2	2.48	0.48
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.95	0.48
1:B:350:THR:HB	1:B:441:LEU:HD22	1.96	0.47
1:A:370:LYS:HG2	1:B:351:LEU:HD13	1.96	0.47
1:D:429:HIS:CD2	1:D:431:ALA:H	2.31	0.47
1:C:377:ILE:HD11	1:C:427:VAL:HG13	1.96	0.47
1:D:318:GLU:HG2	1:D:335:THR:CG2	2.45	0.47
1:B:247:PRO:HA	1:B:250:THR:HG22	1.97	0.47
1:C:312:ASP:HB3	1:C:317:LYS:HD2	1.96	0.47
1:D:311:GLN:HB3	7:D:605:HOH:O	2.14	0.47
1:C:351:LEU:HD22	1:D:347:GLN:HB3	1.96	0.47
1:B:277:TRP:O	1:B:283:GLU:HA	2.14	0.47
1:B:247:PRO:O	1:B:250:THR:HG22	2.16	0.46
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.98	0.46
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.50	0.46
1:C:422:VAL:HG22	1:C:442:SER:HB3	1.99	0.45
1:A:241:PHE:CZ	2:A:502:NAG:H61	2.52	0.45
1:C:278:TYR:HB2	1:C:320:LYS:HD2	1.99	0.45
1:A:371:GLY:HA2	1:A:403:SER:OG	2.17	0.45
1:B:255:ARG:N	1:B:255:ARG:HD2	2.32	0.44
1:A:346:PRO:HB3	1:A:372:PHE:HB3	2.00	0.44
1:C:240:VAL:HG22	1:C:263:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HA	1:C:352:PRO:HD3	1.92	0.43
1:C:250:THR:HG21	1:C:313:TRP:HD1	1.82	0.43
3:D:503:BMA:H2	4:D:506:MAN:O5	2.19	0.43
1:C:384:ASN:HB3	7:C:607:HOH:O	2.19	0.43
1:B:318:GLU:HG2	1:B:335:THR:HG22	2.00	0.42
1:A:258:GLU:HB2	1:A:305:VAL:HG12	2.02	0.42
1:B:266:VAL:HB	1:B:300:TYR:HB2	2.01	0.42
1:D:260:THR:HG21	2:D:505:NAG:H61	2.01	0.42
1:B:271:PRO:O	1:B:273:VAL:HG23	2.19	0.42
1:A:444:SER:O	1:A:445:PRO:C	2.58	0.42
1:B:417:TRP:NE1	1:B:443:LEU:HD13	2.35	0.42
1:C:296:TYR:CD2	6:C:508:FUC:H62	2.55	0.42
1:B:245:PRO:HD3	1:B:259:VAL:HG22	2.01	0.41
1:C:399:ASP:HB3	1:C:401:ASP:OD1	2.20	0.41
1:B:349:CYS:HB3	1:B:368:ALA:HB3	2.02	0.41
1:B:388:GLU:CD	1:B:416:ARG:HH22	2.24	0.41
1:B:436:TYR:CE1	1:B:438:GLN:HG3	2.55	0.41
1:D:261:CYS:HB2	1:D:277:TRP:CZ2	2.55	0.41
1:A:257:PRO:HB2	1:A:308:VAL:HG22	2.03	0.41
1:B:292:ARG:HB2	1:B:300:TYR:HD1	1.86	0.41
1:C:351:LEU:HB2	1:C:366:SER:HB2	2.03	0.41
1:D:406:LEU:HD12	1:D:406:LEU:C	2.42	0.40
1:A:397:VAL:HG11	1:B:397:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

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	207/227 (91%)	197 (95%)	9 (4%)	1 (0%)	32	68
1	B	207/227 (91%)	190 (92%)	11 (5%)	6 (3%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	206/227 (91%)	186 (90%)	18 (9%)	2 (1%)	18	51
1	D	207/227 (91%)	197 (95%)	8 (4%)	2 (1%)	18	51
All	All	827/908 (91%)	770 (93%)	46 (6%)	11 (1%)	14	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	B	376	ASP
1	B	254	SER
1	B	310	HIS
1	D	310	HIS
1	D	311	GLN
1	B	292	ARG
1	B	253	ILE
1	B	358	LEU
1	C	297	ASN
1	C	238	PRO

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	194/209 (93%)	176 (91%)	18 (9%)	10	31
1	B	193/209 (92%)	175 (91%)	18 (9%)	10	31
1	C	193/209 (92%)	170 (88%)	23 (12%)	6	18
1	D	193/209 (92%)	172 (89%)	21 (11%)	7	22
All	All	773/836 (92%)	693 (90%)	80 (10%)	8	25

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LYS

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Mol	Chain	Res	Type
1	A	254	SER
1	A	256	THR
1	A	289	THR
1	A	309	LEU
1	A	324	SER
1	A	335	THR
1	A	338	LYS
1	A	354	SER
1	A	356	ASP
1	A	360	LYS
1	A	366	SER
1	A	367	CYS
1	A	370	LYS
1	A	392	LYS
1	A	396	PRO
1	A	398	LEU
1	A	437	THR
1	B	239	SER
1	B	251	LEU
1	B	255	ARG
1	B	260	THR
1	B	289	THR
1	B	309	LEU
1	B	310	HIS
1	B	312	ASP
1	B	328	LEU
1	B	335	THR
1	B	351	LEU
1	B	360	LYS
1	B	361	ASN
1	B	366	SER
1	B	370	LYS
1	B	403	SER
1	B	411	THR
1	B	418	GLN
1	C	250	THR
1	C	252	MET
1	C	253	ILE
1	C	254	SER
1	C	264	VAL
1	C	269	GLU
1	C	270	ASP

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Mol	Chain	Res	Type
1	C	274	LYS
1	C	282	VAL
1	C	285	HIS
1	C	309	LEU
1	C	311	GLN
1	C	320	LYS
1	C	336	ILE
1	C	342	GLN
1	C	349	CYS
1	C	354	SER
1	C	360	LYS
1	C	366	SER
1	C	370	LYS
1	C	382	GLU
1	C	413	ASP
1	C	421	ASN
1	D	255	ARG
1	D	272	GLU
1	D	288	LYS
1	D	289	THR
1	D	290	LYS
1	D	310	HIS
1	D	315	ASN
1	D	326	LYS
1	D	337	SER
1	D	338	LYS
1	D	340	LYS
1	D	349	CYS
1	D	357	GLU
1	D	360	LYS
1	D	370	LYS
1	D	382	GLU
1	D	392	LYS
1	D	400	SER
1	D	415	SER
1	D	426	SER
1	D	437	THR

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

Mol	Chain	Res	Type
1	B	361	ASN

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Mol	Chain	Res	Type
1	C	276	ASN
1	C	347	GLN
1	C	421	ASN
1	D	276	ASN
1	D	311	GLN
1	D	429	HIS
1	D	434	ASN
1	D	435	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	501	1,2,6	14,14,15	0.26	0	15,19,21	0.73	1 (6%)
2	NAG	A	502	3,2	14,14,15	0.32	0	15,19,21	0.97	1 (6%)
3	BMA	A	503	2,4	11,11,12	0.44	0	13,15,17	0.76	0
4	MAN	A	504	3,2	11,11,12	0.36	0	13,15,17	0.91	2 (15%)
2	NAG	A	505	5,4	14,14,15	0.24	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	506	3,2	11,11,12	0.73	1 (9%)	13,15,17	1.89	2 (15%)
5	GAL	A	507	2	11,11,12	0.46	0	13,15,17	0.75	0
6	FUC	A	508	2	9,10,11	0.48	0	13,14,16	0.93	1 (7%)
2	NAG	A	509	4	14,14,15	0.38	0	15,19,21	1.69	2 (13%)
2	NAG	B	501	1,2,6	14,14,15	0.29	0	15,19,21	0.83	1 (6%)
2	NAG	B	502	3,2	14,14,15	0.34	0	15,19,21	0.71	1 (6%)
3	BMA	B	503	2,4	11,11,12	0.27	0	13,15,17	0.90	1 (7%)
4	MAN	B	504	3,2	11,11,12	0.57	0	13,15,17	1.09	2 (15%)
2	NAG	B	505	5,4	14,14,15	0.33	0	15,19,21	1.15	2 (13%)
4	MAN	B	506	3,2	11,11,12	0.51	0	13,15,17	1.43	2 (15%)
5	GAL	B	507	2	11,11,12	0.44	0	13,15,17	0.69	0
6	FUC	B	508	2	9,10,11	0.50	0	13,14,16	0.95	1 (7%)
2	NAG	B	509	4	14,14,15	0.25	0	15,19,21	1.29	2 (13%)
2	NAG	C	501	1,2,6	14,14,15	0.28	0	15,19,21	1.07	2 (13%)
2	NAG	C	502	3,2	14,14,15	0.37	0	15,19,21	0.67	0
3	BMA	C	503	2,4	11,11,12	0.51	0	13,15,17	0.71	0
4	MAN	C	504	3,2	11,11,12	0.39	0	13,15,17	1.18	1 (7%)
2	NAG	C	505	5,4	14,14,15	0.27	0	15,19,21	1.75	2 (13%)
4	MAN	C	506	3,2	11,11,12	0.43	0	13,15,17	0.84	1 (7%)
5	GAL	C	507	2	11,11,12	0.39	0	13,15,17	0.62	0
6	FUC	C	508	2	9,10,11	0.41	0	13,14,16	1.46	2 (15%)
2	NAG	C	509	4	14,14,15	0.35	0	15,19,21	0.61	0
2	NAG	D	501	1,2,6	14,14,15	0.29	0	15,19,21	0.62	0
2	NAG	D	502	3,2	14,14,15	0.29	0	15,19,21	0.58	0
3	BMA	D	503	2,4	11,11,12	0.37	0	13,15,17	0.74	0
4	MAN	D	504	3,2	11,11,12	0.34	0	13,15,17	0.93	1 (7%)
2	NAG	D	505	5,4	14,14,15	0.37	0	15,19,21	1.03	1 (6%)
4	MAN	D	506	3,2	11,11,12	0.61	0	13,15,17	1.74	2 (15%)
5	GAL	D	507	2	11,11,12	0.50	0	13,15,17	0.73	0
6	FUC	D	508	2	9,10,11	0.37	0	13,14,16	0.80	1 (7%)
2	NAG	D	509	4	14,14,15	0.31	0	15,19,21	0.77	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1,2,6	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	A	505	5,4	-	0/6/23/26	0/1/1/1
4	MAN	A	506	3,2	-	0/2/19/22	0/1/1/1
5	GAL	A	507	2	-	0/2/19/22	0/1/1/1
6	FUC	A	508	2	-	0/0/17/20	0/1/1/1
2	NAG	A	509	4	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,2,6	-	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	505	5,4	-	0/6/23/26	0/1/1/1
4	MAN	B	506	3,2	-	0/2/19/22	0/1/1/1
5	GAL	B	507	2	-	0/2/19/22	0/1/1/1
6	FUC	B	508	2	-	0/0/17/20	0/1/1/1
2	NAG	B	509	4	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1,2,6	-	0/6/23/26	0/1/1/1
2	NAG	C	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	C	505	5,4	-	0/6/23/26	0/1/1/1
4	MAN	C	506	3,2	-	0/2/19/22	0/1/1/1
5	GAL	C	507	2	-	0/2/19/22	0/1/1/1
6	FUC	C	508	2	-	0/0/17/20	0/1/1/1
2	NAG	C	509	4	-	0/6/23/26	0/1/1/1
2	NAG	D	501	1,2,6	-	0/6/23/26	0/1/1/1
2	NAG	D	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	D	504	3,2	-	0/2/19/22	0/1/1/1
2	NAG	D	505	5,4	-	0/6/23/26	0/1/1/1
4	MAN	D	506	3,2	-	0/2/19/22	0/1/1/1
5	GAL	D	507	2	-	0/2/19/22	0/1/1/1
6	FUC	D	508	2	-	0/0/17/20	0/1/1/1
2	NAG	D	509	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	MAN	C1-C2	2.00	1.56	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	505	NAG	O5-C1-C2	-4.67	104.98	111.47
2	B	509	NAG	O5-C1-C2	-3.75	106.25	111.47
2	A	502	NAG	O5-C1-C2	-3.17	107.06	111.47
2	D	505	NAG	O5-C1-C2	-2.92	107.41	111.47
2	A	505	NAG	O5-C1-C2	-2.67	107.76	111.47
2	B	505	NAG	O5-C1-C2	-2.51	107.98	111.47
2	D	509	NAG	C1-C2-N2	-2.24	106.67	110.49
2	A	501	NAG	C1-C2-N2	-2.05	106.99	110.49
2	C	501	NAG	O5-C1-C2	-2.01	108.67	111.47
4	A	504	MAN	C1-C2-C3	2.01	112.20	109.65
2	B	502	NAG	C1-O5-C5	2.02	114.95	112.17
4	B	504	MAN	C1-O5-C5	2.04	114.98	112.17
2	A	509	NAG	C3-C4-C5	2.04	113.82	110.22
4	C	506	MAN	C1-O5-C5	2.07	115.02	112.17
6	D	508	FUC	C1-O5-C5	2.21	117.28	112.39
2	B	505	NAG	C1-O5-C5	2.21	115.22	112.17
2	C	501	NAG	C1-C2-N2	2.25	114.33	110.49
6	A	508	FUC	C1-O5-C5	2.29	117.45	112.39
4	A	504	MAN	C1-O5-C5	2.41	115.48	112.17
4	B	506	MAN	C1-C2-C3	2.42	112.72	109.65
2	B	501	NAG	C1-O5-C5	2.53	115.65	112.17
6	B	508	FUC	C1-O5-C5	2.55	118.04	112.39
2	B	509	NAG	C1-O5-C5	2.57	115.71	112.17
4	C	504	MAN	C1-O5-C5	2.77	115.99	112.17
3	B	503	BMA	C1-O5-C5	2.80	116.02	112.17
6	C	508	FUC	C1-O5-C5	2.80	118.58	112.39
4	B	504	MAN	C1-C2-C3	2.85	113.27	109.65
4	D	504	MAN	C1-O5-C5	3.10	116.44	112.17
4	B	506	MAN	O2-C2-C3	3.14	116.35	110.17
4	A	506	MAN	C1-C2-C3	3.40	113.97	109.65
4	D	506	MAN	C1-C2-C3	3.56	114.16	109.65
2	C	505	NAG	C1-C2-N2	3.62	116.68	110.49
6	C	508	FUC	C3-C4-C5	3.72	115.52	109.68
4	D	506	MAN	C1-O5-C5	3.78	117.38	112.17
4	A	506	MAN	C1-O5-C5	4.61	118.52	112.17
2	A	509	NAG	C1-O5-C5	5.41	119.62	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	NAG	1	0
6	C	508	FUC	1	0
3	D	503	BMA	1	0
2	D	505	NAG	1	0
4	D	506	MAN	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	209/227 (92%)	-0.11	0 100 100	59, 80, 110, 127	0
1	B	209/227 (92%)	0.28	7 (3%) 47 40	56, 97, 143, 166	0
1	C	208/227 (91%)	0.38	14 (6%) 19 14	60, 103, 163, 178	0
1	D	209/227 (92%)	-0.04	0 100 100	58, 81, 116, 137	0
All	All	835/908 (91%)	0.13	21 (2%) 58 53	56, 86, 145, 178	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	SER	5.4
1	B	310	HIS	5.3
1	C	275	PHE	5.1
1	C	276	ASN	4.3
1	C	277	TRP	4.2
1	B	296	TYR	3.6
1	C	239	SER	3.2
1	B	323	VAL	3.1
1	C	278	TYR	3.1
1	C	273	VAL	2.8
1	C	264	VAL	2.5
1	C	333	GLU	2.4
1	C	321	CYS	2.4
1	B	236	GLY	2.3
1	B	302	VAL	2.2
1	C	274	LYS	2.2
1	C	284	VAL	2.2
1	B	262	VAL	2.2
1	B	266	VAL	2.2
1	C	238	PRO	2.1
1	C	323	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no 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
2	NAG	A	505	14/15	0.97	0.19	-0.44	104,107,114,114	0
5	GAL	C	507	11/12	0.92	0.16	-0.60	103,111,114,114	0
5	GAL	A	507	11/12	0.95	0.16	-0.71	104,109,114,115	0
2	NAG	A	501	14/15	0.96	0.14	-0.79	98,110,118,120	0
2	NAG	B	501	14/15	0.89	0.19	-1.00	128,137,142,145	0
5	GAL	D	507	11/12	0.97	0.17	-1.04	91,96,98,99	0
2	NAG	B	505	14/15	0.92	0.14	-1.23	118,120,124,124	0
2	NAG	C	505	14/15	0.97	0.11	-1.44	101,104,106,107	0
5	GAL	B	507	11/12	0.94	0.12	-1.79	129,132,136,137	0
2	NAG	A	502	14/15	0.98	0.14	-1.94	85,91,97,98	0
2	NAG	C	502	14/15	0.94	0.20	-2.11	120,130,137,137	0
2	NAG	D	502	14/15	0.96	0.14	-2.22	101,106,108,114	0
2	NAG	D	505	14/15	0.97	0.16	-2.69	98,102,106,107	0
3	BMA	C	503	11/12	0.93	0.11	-	114,130,135,142	0
2	NAG	B	509	14/15	0.91	0.16	-	147,151,154,155	0
4	MAN	D	506	11/12	0.91	0.16	-	140,147,151,153	0
2	NAG	A	509	14/15	0.93	0.21	-	135,145,149,149	0
2	NAG	C	509	14/15	0.90	0.10	-	167,174,177,177	0
4	MAN	B	504	11/12	0.93	0.11	-	121,126,127,129	0
2	NAG	D	509	14/15	0.92	0.14	-	135,141,143,144	0
4	MAN	C	504	11/12	0.96	0.10	-	100,110,115,115	0
3	BMA	B	503	11/12	0.96	0.09	-	115,117,122,128	0
3	BMA	A	503	11/12	0.95	0.12	-	96,102,108,118	0
4	MAN	A	506	11/12	0.90	0.16	-	127,130,135,142	0
4	MAN	D	504	11/12	0.92	0.19	-	112,119,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	D	503	11/12	0.94	0.11	-	114,116,124,132	0
2	NAG	C	501	14/15	0.94	0.18	-	138,146,155,160	0
4	MAN	C	506	11/12	0.92	0.10	-	154,159,160,168	0
4	MAN	B	506	11/12	0.94	0.13	-	135,140,142,145	0
6	FUC	C	508	10/11	0.86	0.19	-	142,146,149,149	0
6	FUC	A	508	10/11	0.93	0.23	-	124,129,134,136	0
6	FUC	B	508	10/11	0.90	0.18	-	142,149,153,156	0
2	NAG	B	502	14/15	0.95	0.10	-	108,113,119,120	0
6	FUC	D	508	10/11	0.92	0.18	-	115,119,123,123	0
4	MAN	A	504	11/12	0.96	0.17	-	105,111,122,123	0
2	NAG	D	501	14/15	0.94	0.13	-	107,111,127,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.