



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 PM GMT

PDB ID : 4Q6Y
Title : Crystal structure of a chemoenzymatic glycoengineered disialylated Fc (di-sFc)
Authors : Ahmed, A.A.; Giddens, J.; Pincetic, A.; Lomino, J.V.; Ravetch, J.V.; Wang, L.X.; Bjorkman, P.J.
Deposited on : 2014-04-23
Resolution : 3.00 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

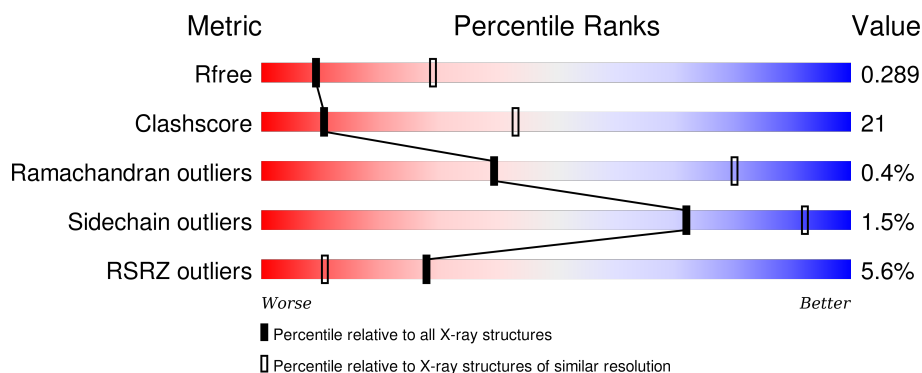
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	221	<div> <div>4%</div> <div>68%</div> <div>25%</div> <div>6%</div> </div>
1	B	221	<div> <div>68%</div> <div>24%</div> <div>7%</div> </div>
1	C	221	<div> <div>10%</div> <div>65%</div> <div>24%</div> <div>10%</div> </div>
1	D	221	<div> <div>6%</div> <div>64%</div> <div>22%</div> <div>12%</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
2	NAG	C	501	-	-	X	-
2	NAG	C	502	-	-	X	-
3	NAG	A	502	-	-	X	-
4	MAN	B	508	-	-	X	-
4	MAN	C	507	-	-	X	-
4	MAN	D	504	-	-	X	-
6	BMA	C	503	-	-	X	-
6	MAN	C	504	X	-	-	-
6	GAL	C	506	-	-	X	-
7	SIA	C	509	-	-	X	-
8	NAG	D	501	X	-	-	-
8	BMA	D	503	-	-	X	-
9	MAN	D	506	X	-	-	-
9	GAL	D	508	-	-	-	X

2 Entry composition [i](#)

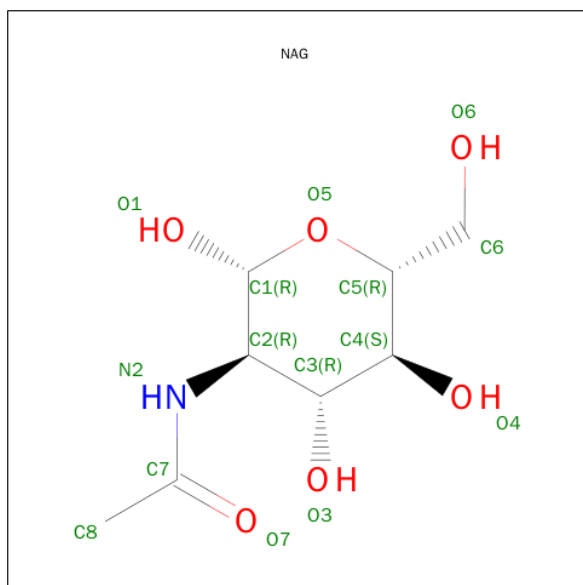
There are 9 unique types of molecules in this entry. The entry contains 6575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	208	Total	C	N	O	S	0	0	0
			1547	985	253	303	6			
1	B	206	Total	C	N	O	S	1	0	0
			1610	1027	269	308	6			
1	C	199	Total	C	N	O	S	0	0	0
			1486	946	244	290	6			
1	D	195	Total	C	N	O	S	1	0	0
			1503	960	250	287	6			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			25	14	1	10		
4	B	2	Total	C	N	O	0	0
			25	14	1	10		
4	C	2	Total	C	N	O	0	0
			25	14	1	10		
4	D	2	Total	C	N	O	0	0
			25	14	1	10		

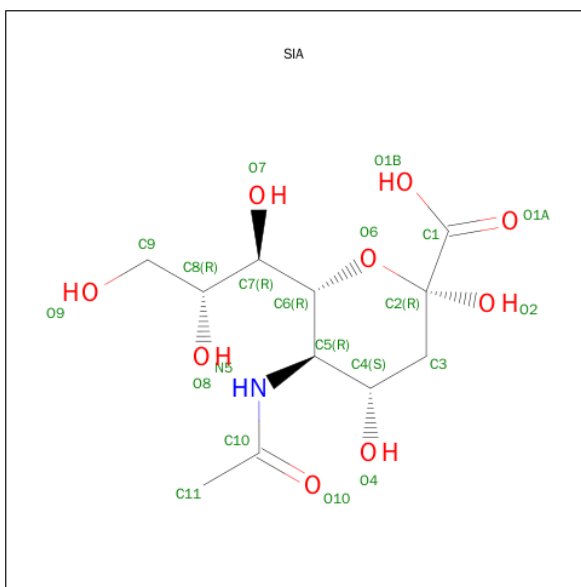
- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			95	53	4	38		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	4	Total	C	N	O	0	0
			47	26	1	20		

- Molecule 7 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



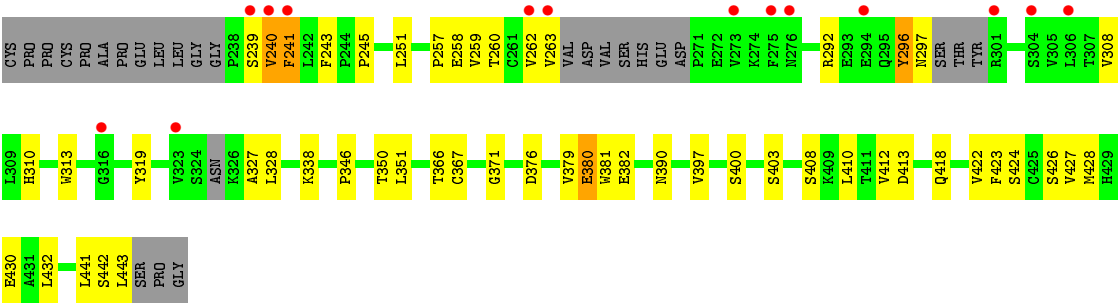
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	3	Total	C	N	O	0	0
			36	20	1	15		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.73Å 154.22Å 66.12Å 90.00° 110.78° 90.00°	Depositor
Resolution (Å)	48.23 – 3.00 48.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.23-3.00) 97.7 (48.23-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX REFINE	Depositor
R, R_{free}	0.260 , 0.280 0.267 , 0.289	Depositor DCC
R_{free} test set	1937 reflections (11.14%)	DCC
Wilson B-factor (Å ²)	71.0	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.3	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19323 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6575	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: MAN, SIA, GAL, BMA, 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	A	0.55	0/1590	0.71	2/2186 (0.1%)
1	B	0.58	0/1655	0.74	0/2261
1	C	0.45	0/1524	0.79	4/2089 (0.2%)
1	D	0.58	1/1544 (0.1%)	0.71	1/2107 (0.0%)
All	All	0.54	1/6313 (0.0%)	0.74	7/8643 (0.1%)

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	1
6	C	1	0
8	D	1	0
9	D	1	0
All	All	3	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	TYR	C-N	5.43	1.46	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	300	TYR	O-C-N	11.77	141.53	122.70
1	C	300	TYR	C-N-CA	-8.65	100.08	121.70
1	C	300	TYR	CA-C-N	-8.64	98.20	117.20
1	A	246	LYS	C-N-CD	5.98	140.96	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	LYS	C-N-CD	5.59	140.13	128.40
1	D	296	TYR	C-N-CA	5.21	134.73	121.70
1	C	441	LEU	CA-CB-CG	5.05	126.91	115.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	504	MAN	C1
8	D	501	NAG	C1
9	D	506	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	296	TYR	Mainchain

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	1547	0	1411	60	14
1	B	1610	0	1535	57	0
1	C	1486	0	1358	61	0
1	D	1503	0	1405	47	0
2	A	14	0	13	2	0
2	C	28	0	26	10	0
3	A	50	0	43	14	0
4	A	25	0	22	3	0
4	B	25	0	22	8	0
4	C	25	0	22	6	0
4	D	25	0	22	7	0
5	B	95	0	80	11	0
6	C	47	0	40	17	0
7	C	20	0	17	7	14
8	D	39	0	33	6	0
9	D	36	0	31	5	0
All	All	6575	0	6080	259	14

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 21.

All (259) 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:297:ASN:HD21	5:B:501:NAG:C1	1.37	1.37
1:C:297:ASN:HD21	2:C:501:NAG:C1	1.38	1.35
1:C:240:VAL:O	1:C:241:PHE:HD1	1.28	1.12
1:B:238:PRO:CG	1:B:328:LEU:HD21	1.80	1.12
1:B:238:PRO:HG2	1:B:328:LEU:HD21	1.23	1.09
1:D:239:SER:O	1:D:240:VAL:HG22	1.52	1.09
1:B:241:PHE:HE2	5:B:503:BMA:C1	1.65	1.09
1:D:240:VAL:HG11	1:D:263:VAL:HA	1.34	1.03
1:C:297:ASN:OD1	1:C:298:SER:N	1.93	1.02
1:A:328:LEU:HD13	1:A:328:LEU:O	1.64	0.98
1:D:240:VAL:HG11	1:D:263:VAL:CA	1.95	0.97
6:C:503:BMA:C3	4:C:507:MAN:C1	2.42	0.97
1:C:240:VAL:C	1:C:241:PHE:HD1	1.68	0.96
1:B:241:PHE:CE2	5:B:503:BMA:C1	2.48	0.95
1:C:240:VAL:O	1:C:241:PHE:CD1	2.19	0.95
6:C:506:GAL:C6	7:C:509:SIA:C1	2.45	0.94
1:D:241:PHE:CZ	4:D:504:MAN:O6	2.21	0.93
1:A:297:ASN:OD1	1:A:298:SER:N	2.01	0.93
1:C:297:ASN:HD22	2:C:501:NAG:C1	1.80	0.92
1:A:328:LEU:O	1:A:328:LEU:CD1	2.18	0.91
1:C:240:VAL:C	1:C:241:PHE:CD1	2.47	0.88
6:C:506:GAL:O6	7:C:509:SIA:C1	2.21	0.88
1:C:266:VAL:HG12	1:C:267:SER:N	1.87	0.88
6:C:503:BMA:O3	4:C:507:MAN:C2	2.21	0.87
8:D:503:BMA:C3	4:D:504:MAN:C1	2.52	0.87
1:D:239:SER:O	1:D:240:VAL:CG2	2.22	0.87
1:B:268:HIS:NE2	1:B:298:SER:O	2.08	0.87
6:C:503:BMA:C1	2:C:502:NAG:HO4	1.87	0.86
1:C:295:GLN:O	1:C:296:TYR:O	1.93	0.86
1:B:295:GLN:O	1:B:297:ASN:OD1	1.93	0.85
1:A:295:GLN:CB	1:A:296:TYR:C	2.45	0.85
1:C:267:SER:OG	1:C:294:GLU:OE1	1.92	0.85
6:C:506:GAL:H62	7:C:509:SIA:C1	2.06	0.85
1:D:241:PHE:CE1	4:D:504:MAN:O6	2.29	0.84
1:C:267:SER:CB	1:C:294:GLU:OE1	2.25	0.84
1:C:285:HIS:N	1:C:286:ASN:HB2	1.93	0.83
1:D:260:THR:HG21	9:D:507:NAG:H61	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:VAL:HB	1:D:262:VAL:O	1.80	0.81
1:D:240:VAL:HG11	1:D:263:VAL:C	2.00	0.81
6:C:506:GAL:HO6	7:C:509:SIA:C2	1.91	0.81
1:A:290:LYS:HD3	1:A:291:PRO:HD2	1.63	0.80
1:C:266:VAL:CG1	1:C:267:SER:N	2.44	0.80
1:A:295:GLN:CB	1:A:296:TYR:O	2.30	0.79
3:A:502:NAG:H5	4:B:508:MAN:O4	1.83	0.78
1:A:298:SER:O	1:A:299:THR:OG1	2.00	0.78
1:A:308:VAL:HG12	1:A:309:LEU:N	2.00	0.77
1:B:240:VAL:C	1:B:241:PHE:HD1	1.88	0.77
2:C:501:NAG:HO4	2:C:502:NAG:C1	1.95	0.76
1:D:258:GLU:HB2	9:D:508:GAL:O3	1.85	0.76
1:C:297:ASN:OD1	1:C:299:THR:N	2.18	0.76
1:C:296:TYR:O	1:C:297:ASN:OD1	2.04	0.76
1:D:240:VAL:C	1:D:241:PHE:CG	2.59	0.75
1:A:328:LEU:HD13	1:A:328:LEU:C	2.07	0.75
2:C:501:NAG:C4	2:C:502:NAG:C1	2.64	0.74
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.74
1:A:240:VAL:O	1:A:241:PHE:HD1	1.70	0.74
5:B:502:NAG:H83	5:B:504:MAN:O4	1.88	0.74
1:B:325:ASN:HB3	1:B:328:LEU:CD1	2.18	0.73
1:A:295:GLN:CB	1:A:296:TYR:CA	2.67	0.73
1:D:240:VAL:O	1:D:241:PHE:CG	2.42	0.73
3:A:503:BMA:C3	4:A:506:MAN:C1	2.68	0.71
1:A:298:SER:C	1:A:299:THR:HG23	2.09	0.71
1:C:278:TYR:CE2	1:C:283:GLU:OE1	2.43	0.71
1:C:351:LEU:HB2	1:C:366:THR:HB	1.72	0.71
2:C:501:NAG:O4	2:C:502:NAG:C2	2.39	0.70
3:A:502:NAG:C5	4:B:508:MAN:O4	2.38	0.70
1:D:240:VAL:CG1	1:D:263:VAL:HA	2.16	0.70
6:C:506:GAL:C6	7:C:509:SIA:O1B	2.38	0.70
1:D:260:THR:HG21	9:D:507:NAG:C6	2.21	0.70
1:C:266:VAL:CG1	1:C:267:SER:H	2.04	0.70
1:B:325:ASN:HB3	1:B:328:LEU:HD12	1.75	0.69
1:B:414:LYS:NZ	1:D:413:ASP:OD1	2.26	0.69
1:C:422:VAL:HG22	1:C:442:SER:HB2	1.75	0.69
6:C:503:BMA:H3	4:C:507:MAN:C1	2.23	0.68
1:A:241:PHE:CE2	3:A:502:NAG:H61	2.29	0.68
1:A:308:VAL:CG1	1:A:309:LEU:N	2.57	0.68
1:C:285:HIS:H	1:C:286:ASN:HB2	1.58	0.67
1:B:342:GLN:H	1:B:342:GLN:CD	1.97	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:BMA:HO3	4:A:506:MAN:C1	2.01	0.67
1:D:240:VAL:C	1:D:241:PHE:CD2	2.68	0.67
1:D:239:SER:C	1:D:240:VAL:HG22	2.14	0.67
1:A:306:LEU:HD23	1:A:307:THR:O	1.95	0.67
1:C:346:PRO:HB3	1:C:372:PHE:HB3	1.77	0.67
1:A:241:PHE:HE2	3:A:502:NAG:H61	1.60	0.67
8:D:503:BMA:O6	9:D:506:MAN:O5	2.13	0.66
1:A:290:LYS:HD3	1:A:291:PRO:CD	2.24	0.66
1:B:297:ASN:N	1:B:297:ASN:OD1	2.27	0.66
1:C:297:ASN:CG	1:C:298:SER:H	1.96	0.66
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.32	0.65
1:B:342:GLN:OE1	1:B:342:GLN:N	2.22	0.64
1:D:327:ALA:C	1:D:328:LEU:HD12	2.17	0.64
3:A:502:NAG:O6	4:B:508:MAN:H5	1.97	0.64
1:C:285:HIS:CB	1:C:286:ASN:HA	2.26	0.64
1:C:278:TYR:CZ	1:C:283:GLU:OE1	2.51	0.63
1:C:383:SER:HB2	1:C:388:GLU:OE2	1.99	0.63
6:C:503:BMA:H2	4:C:507:MAN:H5	1.81	0.63
1:B:259:VAL:HG23	1:B:308:VAL:HG21	1.81	0.62
1:A:295:GLN:CB	1:A:296:TYR:HA	2.28	0.62
1:B:346:PRO:HG2	1:B:432:LEU:HD21	1.82	0.62
1:A:240:VAL:O	1:A:241:PHE:CD1	2.51	0.62
5:B:503:BMA:C3	4:B:508:MAN:C1	2.78	0.61
1:B:342:GLN:HG2	1:B:342:GLN:O	2.01	0.61
1:B:325:ASN:CB	1:B:328:LEU:HD12	2.30	0.60
1:A:299:THR:C	1:A:300:TYR:HD2	2.04	0.60
8:D:503:BMA:O3	4:D:504:MAN:C2	2.50	0.60
1:C:388:GLU:HG3	1:C:389:ASN:H	1.66	0.60
1:A:295:GLN:HA	1:A:299:THR:O	2.02	0.59
1:A:290:LYS:HB2	1:A:303:VAL:O	2.02	0.59
1:C:240:VAL:HG12	1:C:241:PHE:N	2.17	0.59
1:C:239:SER:OG	1:C:264:VAL:CG2	2.50	0.59
6:C:503:BMA:O3	4:C:507:MAN:C3	2.51	0.59
1:C:383:SER:CB	1:C:388:GLU:OE2	2.51	0.59
1:A:328:LEU:HD11	1:A:330:ALA:O	2.02	0.58
1:D:382:GLU:HG2	1:D:424:SER:HB2	1.85	0.58
1:A:298:SER:O	1:A:299:THR:CB	2.49	0.58
1:D:241:PHE:HZ	4:D:504:MAN:O6	1.82	0.58
1:A:299:THR:O	1:A:300:TYR:HD2	1.86	0.58
1:B:297:ASN:HD22	5:B:501:NAG:C1	2.07	0.57
1:D:260:THR:CG2	9:D:507:NAG:H61	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:PHE:CD2	1:D:241:PHE:N	2.72	0.57
1:C:260:THR:HG23	1:C:303:VAL:CG1	2.35	0.57
1:C:377:ILE:HG13	1:C:429:HIS:HB2	1.86	0.57
1:C:257:PRO:HG2	1:C:308:VAL:O	2.04	0.57
1:C:284:VAL:HB	1:C:286:ASN:HB2	1.86	0.57
1:B:265:ASP:HA	1:B:299:THR:HG21	1.87	0.56
1:C:412:VAL:HG11	1:C:423:PHE:CE1	2.41	0.56
1:B:241:PHE:HD1	1:B:241:PHE:N	2.02	0.56
1:C:394:THR:HA	1:D:397:VAL:HG21	1.87	0.56
6:C:506:GAL:H62	7:C:509:SIA:O1B	2.04	0.55
1:A:297:ASN:CG	1:A:298:SER:H	2.10	0.55
1:B:276:ASN:HB2	1:B:322:LYS:HB3	1.89	0.55
1:B:241:PHE:CD1	1:B:241:PHE:N	2.73	0.55
1:B:246:LYS:CD	5:B:506:GAL:O4	2.55	0.55
1:A:390:ASN:ND2	1:A:390:ASN:O	2.40	0.55
1:C:292:ARG:HB3	1:C:302:VAL:HG22	1.88	0.54
1:B:246:LYS:HD3	5:B:506:GAL:O4	2.08	0.54
1:C:262:VAL:HG22	1:C:303:VAL:HG22	1.90	0.54
8:D:503:BMA:H3	4:D:504:MAN:C1	2.36	0.54
8:D:503:BMA:HO3	4:D:504:MAN:C1	2.14	0.54
1:B:344:ARG:HH11	1:B:403:SER:HB3	1.71	0.54
6:C:503:BMA:O3	4:C:507:MAN:H3	2.07	0.54
2:A:501:NAG:C4	3:A:502:NAG:C1	2.82	0.54
1:B:266:VAL:CG2	1:B:300:TYR:HB2	2.38	0.54
2:C:501:NAG:HO3	2:C:502:NAG:C1	2.21	0.53
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.89	0.53
1:D:251:LEU:HD13	1:D:428:MET:O	2.09	0.53
1:B:238:PRO:CD	1:B:328:LEU:HD21	2.37	0.52
3:A:503:BMA:O3	4:A:506:MAN:C2	2.50	0.52
1:B:280:ASP:OD2	1:B:317:LYS:HD2	2.08	0.52
1:B:242:LEU:HD23	1:B:336:ILE:HB	1.92	0.51
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.45	0.51
1:A:240:VAL:C	1:A:241:PHE:CD1	2.83	0.51
2:A:501:NAG:HO4	3:A:502:NAG:C1	2.16	0.51
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.45	0.51
1:A:325:ASN:HB3	1:A:328:LEU:HB3	1.93	0.51
1:A:241:PHE:HE2	3:A:502:NAG:C6	2.24	0.51
1:D:308:VAL:HG22	1:D:319:TYR:CE1	2.46	0.50
1:A:382:GLU:HA	1:A:387:PRO:HA	1.93	0.50
1:A:328:LEU:O	1:A:328:LEU:HD12	2.07	0.50
1:A:350:THR:HB	1:A:441:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:VAL:O	1:D:241:PHE:CD1	2.64	0.49
2:C:501:NAG:O3	2:C:502:NAG:C1	2.61	0.49
1:A:377:ILE:HG13	1:A:429:HIS:HB2	1.93	0.49
1:C:241:PHE:N	1:C:241:PHE:CD1	2.74	0.49
6:C:504:MAN:H3	2:C:502:NAG:O3	2.12	0.49
1:D:371:GLY:HA2	1:D:403:SER:OG	2.13	0.49
1:D:245:PRO:HD3	1:D:259:VAL:HG12	1.94	0.49
1:B:325:ASN:HB3	1:B:328:LEU:HG	1.95	0.48
1:A:298:SER:O	1:A:299:THR:HG23	2.13	0.48
1:A:308:VAL:CG1	1:A:319:TYR:OH	2.61	0.48
1:C:243:PHE:CD2	6:C:505:NAG:H5	2.49	0.48
1:A:328:LEU:CD1	1:A:330:ALA:C	2.82	0.48
1:C:266:VAL:HG13	1:C:267:SER:H	1.79	0.48
1:C:260:THR:CG2	1:C:303:VAL:CG1	2.91	0.48
3:A:502:NAG:C5	4:B:508:MAN:HO4	2.26	0.48
1:A:328:LEU:C	1:A:328:LEU:CD1	2.75	0.48
1:C:392:LYS:NZ	1:D:400:SER:OG	2.44	0.48
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.96	0.47
1:A:249:ASP:OD1	1:A:255:ARG:NE	2.43	0.47
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.47
3:A:502:NAG:O6	4:B:508:MAN:O4	2.27	0.47
1:B:325:ASN:N	1:B:328:LEU:HD12	2.29	0.47
1:D:346:PRO:HG2	1:D:432:LEU:HD21	1.96	0.47
1:C:238:PRO:HB3	1:C:265:ASP:HB2	1.97	0.47
1:D:422:VAL:HG22	1:D:442:SER:HB2	1.96	0.46
5:B:503:BMA:O3	4:B:508:MAN:C2	2.60	0.46
1:B:372:PHE:CD1	1:B:377:ILE:HD12	2.51	0.46
1:A:293:GLU:HA	1:A:294:GLU:HA	1.67	0.46
1:A:290:LYS:CD	1:A:291:PRO:HD2	2.38	0.46
1:D:379:VAL:HG22	1:D:427:VAL:HG22	1.98	0.46
1:B:308:VAL:HG13	1:B:319:TYR:OH	2.16	0.45
1:A:428:MET:HG2	1:A:436:TYR:HD2	1.80	0.45
1:B:241:PHE:CE2	5:B:502:NAG:H4	2.51	0.45
1:B:325:ASN:HB3	1:B:328:LEU:CG	2.46	0.45
7:C:509:SIA:H7	7:C:509:SIA:C10	2.47	0.45
1:C:277:TRP:HB2	1:C:284:VAL:HG23	1.98	0.45
1:A:267:SER:OG	1:A:270:ASP:HB2	2.17	0.45
1:A:253:ILE:HG22	1:A:253:ILE:O	2.17	0.45
1:B:360:LYS:O	1:B:414:LYS:HE2	2.17	0.45
1:A:245:PRO:HD2	1:A:313:TRP:CZ2	2.51	0.45
1:C:338:LYS:HD2	1:C:430:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:CB	1:B:328:LEU:CD1	2.91	0.45
1:C:379:VAL:HG21	1:C:406:LEU:HD11	1.98	0.45
1:D:243:PHE:CZ	8:D:503:BMA:H5	2.52	0.44
1:A:409:LYS:NZ	1:B:399:ASP:OD2	2.50	0.44
1:B:240:VAL:C	1:B:241:PHE:CD1	2.79	0.44
1:B:249:ASP:O	1:B:310:HIS:HE1	2.01	0.44
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.52	0.44
1:A:339:ALA:HB3	1:A:374:PRO:HB3	2.00	0.44
1:A:311:GLN:OE1	1:A:311:GLN:N	2.47	0.44
1:C:336:ILE:HD12	1:C:336:ILE:HA	1.87	0.44
1:B:289:THR:HG22	1:B:290:LYS:O	2.18	0.44
1:D:418:GLN:HA	1:D:443:LEU:HD22	2.00	0.43
1:B:346:PRO:HB3	1:B:372:PHE:HB3	2.01	0.43
1:D:367:CYS:HB3	1:D:408:SER:HB3	1.99	0.43
1:C:243:PHE:CG	6:C:505:NAG:H5	2.52	0.43
1:C:346:PRO:CB	1:C:372:PHE:HB3	2.47	0.43
1:D:257:PRO:HD3	1:D:310:HIS:CE1	2.54	0.43
1:D:380:GLU:HG2	1:D:426:SER:OG	2.19	0.43
1:B:241:PHE:HE2	5:B:503:BMA:C2	2.25	0.43
1:C:293:GLU:O	1:C:294:GLU:HB2	2.20	0.42
1:A:308:VAL:HG11	1:A:319:TYR:OH	2.20	0.42
1:B:344:ARG:NH1	1:B:403:SER:HB3	2.33	0.42
1:C:342:GLN:HA	1:C:343:PRO:HD3	1.82	0.42
1:C:267:SER:HB3	1:C:294:GLU:OE1	2.14	0.42
1:D:308:VAL:HG11	1:D:313:TRP:HB2	2.01	0.42
1:B:309:LEU:HD12	1:B:312:ASP:OD2	2.20	0.42
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.19	0.42
1:A:412:VAL:HG11	1:A:423:PHE:CE1	2.53	0.42
1:C:239:SER:OG	1:C:264:VAL:HG22	2.19	0.42
1:D:442:SER:OG	1:D:443:LEU:N	2.53	0.42
1:C:383:SER:HB3	1:C:388:GLU:OE2	2.19	0.42
1:A:320:LYS:HD2	1:A:333:GLU:OE1	2.19	0.42
1:D:338:LYS:HD2	1:D:430:GLU:OE1	2.20	0.42
1:D:351:LEU:HB2	1:D:366:THR:HB	2.02	0.42
1:A:299:THR:O	1:A:300:TYR:CD2	2.70	0.42
1:C:370:LYS:HB2	1:C:370:LYS:HE2	1.81	0.42
1:B:296:TYR:O	1:B:296:TYR:CG	2.70	0.42
1:D:327:ALA:O	1:D:328:LEU:HD12	2.20	0.41
1:D:350:THR:HB	1:D:441:LEU:HD22	2.01	0.41
1:B:279:VAL:HG23	1:B:279:VAL:O	2.19	0.41
3:A:502:NAG:O6	4:B:508:MAN:C5	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:VAL:CG1	1:D:263:VAL:C	2.82	0.41
1:C:266:VAL:HB	1:C:300:TYR:CB	2.50	0.41
1:C:240:VAL:CG1	1:C:241:PHE:N	2.83	0.41
1:C:246:LYS:O	1:C:250:THR:HG23	2.20	0.41
1:C:241:PHE:HE2	6:C:503:BMA:C1	2.33	0.41
1:C:241:PHE:CE2	2:C:502:NAG:H4	2.56	0.41
1:A:298:SER:O	1:A:299:THR:CG2	2.69	0.41
1:C:284:VAL:HB	1:C:286:ASN:CB	2.51	0.41
1:B:342:GLN:HA	1:B:343:PRO:HD3	1.79	0.41
1:B:292:ARG:HD2	1:B:300:TYR:CD1	2.56	0.41
1:A:260:THR:HG22	1:A:262:VAL:HG23	2.02	0.41
1:B:294:GLU:HB3	1:B:300:TYR:CD1	2.56	0.41
1:D:390:ASN:O	1:D:410:LEU:HD12	2.21	0.41
1:A:351:LEU:HD23	1:B:354:SER:HB2	2.02	0.40
1:A:328:LEU:CD1	1:A:330:ALA:O	2.67	0.40
1:B:325:ASN:H	1:B:328:LEU:HD12	1.86	0.40
1:D:412:VAL:HG11	1:D:423:PHE:CE1	2.56	0.40

All (14) 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)
1:A:286:ASN:CG	7:C:509:SIA:N5[2_445]	1.08	1.12
1:A:286:ASN:ND2	7:C:509:SIA:N5[2_445]	1.41	0.79
1:A:286:ASN:OD1	7:C:509:SIA:C6[2_445]	1.46	0.74
1:A:286:ASN:ND2	7:C:509:SIA:C4[2_445]	1.51	0.69
1:A:286:ASN:ND2	7:C:509:SIA:O4[2_445]	1.54	0.66
1:A:286:ASN:ND2	7:C:509:SIA:C5[2_445]	1.60	0.60
1:A:286:ASN:OD1	7:C:509:SIA:C5[2_445]	1.60	0.60
1:A:286:ASN:CG	7:C:509:SIA:C5[2_445]	1.62	0.58
1:A:306:LEU:CD2	7:C:509:SIA:C11[2_445]	1.75	0.45
1:A:286:ASN:CB	7:C:509:SIA:N5[2_445]	1.78	0.42
1:A:286:ASN:OD1	7:C:509:SIA:N5[2_445]	1.91	0.29
1:A:286:ASN:CG	7:C:509:SIA:C4[2_445]	1.97	0.23
1:A:286:ASN:OD1	7:C:509:SIA:C4[2_445]	2.03	0.17
1:A:306:LEU:CG	7:C:509:SIA:C11[2_445]	2.05	0.15

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/221 (93%)	191 (93%)	14 (7%)	1 (0%)	34	76
1	B	202/221 (91%)	194 (96%)	8 (4%)	0	100	100
1	C	193/221 (87%)	180 (93%)	12 (6%)	1 (0%)	34	76
1	D	187/221 (85%)	179 (96%)	7 (4%)	1 (0%)	34	76
All	All	788/884 (89%)	744 (94%)	41 (5%)	3 (0%)	39	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	296	TYR
1	D	240	VAL
1	A	299	THR

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	166/204 (81%)	164 (99%)	2 (1%)	78	94
1	B	182/204 (89%)	179 (98%)	3 (2%)	70	92
1	C	160/204 (78%)	160 (100%)	0	100	100
1	D	164/204 (80%)	159 (97%)	5 (3%)	48	83
All	All	672/816 (82%)	662 (98%)	10 (2%)	72	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	384	ASN
1	B	297	ASN
1	B	356	ASP
1	B	439	LYS
1	D	241	PHE
1	D	292	ARG
1	D	297	ASN
1	D	376	ASP
1	D	380	GLU

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

Mol	Chain	Res	Type
1	A	325	ASN
1	B	419	GLN
1	C	325	ASN

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 ⓘ

29 carbohydrates 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	502	3,2	14,14,15	1.55	2 (14%)	15,19,21	1.13	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	503	3,4	11,11,12	0.61	0	14,15,17	1.63	3 (21%)
3	MAN	A	504	3	11,11,12	0.78	0	14,15,17	1.47	1 (7%)
3	NAG	A	505	3	14,14,15	1.56	2 (14%)	15,19,21	1.14	2 (13%)
4	MAN	A	506	3,4	11,11,12	1.62	2 (18%)	14,15,17	0.98	1 (7%)
4	NAG	A	507	4	14,14,15	0.47	0	15,19,21	1.05	1 (6%)
5	NAG	B	501	1,5	14,14,15	0.65	0	15,19,21	1.44	3 (20%)
5	NAG	B	502	5	14,14,15	0.73	0	15,19,21	1.36	3 (20%)
5	BMA	B	503	5,4	11,11,12	0.51	0	14,15,17	1.96	4 (28%)
5	MAN	B	504	5	11,11,12	0.88	1 (9%)	14,15,17	1.97	1 (7%)
5	NAG	B	505	5	14,14,15	0.73	0	15,19,21	0.64	0
5	GAL	B	506	5	11,11,12	1.46	2 (18%)	14,15,17	1.01	1 (7%)
5	SIA	B	507	5	16,20,21	1.92	6 (37%)	18,28,31	1.46	3 (16%)
4	MAN	B	508	5,4	11,11,12	1.62	2 (18%)	14,15,17	0.97	1 (7%)
4	NAG	B	509	4	14,14,15	0.45	0	15,19,21	1.24	1 (6%)
6	BMA	C	503	2,4,6	11,11,12	0.93	1 (9%)	14,15,17	2.72	5 (35%)
6	MAN	C	504	6	11,11,12	1.63	2 (18%)	14,15,17	0.98	1 (7%)
6	NAG	C	505	6	14,14,15	0.74	0	15,19,21	0.64	0
6	GAL	C	506	7,6	11,11,12	1.45	2 (18%)	14,15,17	1.01	1 (7%)
4	MAN	C	507	4,6	11,11,12	1.63	2 (18%)	14,15,17	0.97	1 (7%)
4	NAG	C	508	4	14,14,15	1.54	2 (14%)	15,19,21	1.14	2 (13%)
8	NAG	D	501	1,8	14,14,15	0.64	0	15,19,21	1.44	2 (13%)
8	NAG	D	502	8	14,14,15	1.55	2 (14%)	15,19,21	1.14	2 (13%)
8	BMA	D	503	9,8,4	11,11,12	0.96	1 (9%)	14,15,17	1.66	3 (21%)
4	MAN	D	504	8,4	11,11,12	1.63	2 (18%)	14,15,17	0.97	1 (7%)
4	NAG	D	505	4	14,14,15	0.44	0	15,19,21	1.23	1 (6%)
9	MAN	D	506	9,8	11,11,12	1.62	2 (18%)	14,15,17	0.98	1 (7%)
9	NAG	D	507	9	14,14,15	0.73	0	15,19,21	0.64	0
9	GAL	D	508	9	11,11,12	0.68	0	14,15,17	0.84	1 (7%)

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	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	504	3	-	0/2/19/22	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1
4	MAN	A	506	3,4	-	0/2/19/22	0/1/1/1
4	NAG	A	507	4	-	0/6/23/26	0/1/1/1
5	NAG	B	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	502	5	-	0/6/23/26	0/1/1/1
5	BMA	B	503	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	504	5	-	0/2/19/22	0/1/1/1
5	NAG	B	505	5	-	0/6/23/26	0/1/1/1
5	GAL	B	506	5	-	0/2/19/22	0/1/1/1
5	SIA	B	507	5	-	0/14/34/38	0/1/1/1
4	MAN	B	508	5,4	-	0/2/19/22	0/1/1/1
4	NAG	B	509	4	-	0/6/23/26	0/1/1/1
6	BMA	C	503	2,4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	504	6	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	C	505	6	-	0/6/23/26	0/1/1/1
6	GAL	C	506	7,6	-	0/2/19/22	0/1/1/1
4	MAN	C	507	4,6	-	0/2/19/22	0/1/1/1
4	NAG	C	508	4	-	0/6/23/26	0/1/1/1
8	NAG	D	501	1,8	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	D	502	8	-	0/6/23/26	0/1/1/1
8	BMA	D	503	9,8,4	-	0/2/19/22	0/1/1/1
4	MAN	D	504	8,4	-	0/2/19/22	0/1/1/1
4	NAG	D	505	4	-	0/6/23/26	0/1/1/1
9	MAN	D	506	9,8	1/1/4/5	0/2/19/22	0/1/1/1
9	NAG	D	507	9	-	0/6/23/26	0/1/1/1
9	GAL	D	508	9	-	0/2/19/22	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	504	MAN	C2-C3	-3.30	1.48	1.52
4	D	504	MAN	C2-C3	-3.26	1.48	1.52
4	C	507	MAN	C2-C3	-3.26	1.48	1.52
4	A	506	MAN	C2-C3	-3.26	1.48	1.52
4	B	508	MAN	C2-C3	-3.25	1.48	1.52
9	D	506	MAN	C2-C3	-3.25	1.48	1.52
5	B	506	GAL	C2-C3	-2.74	1.48	1.52
6	C	506	GAL	C2-C3	-2.73	1.48	1.52
8	D	503	BMA	O6-C6	-2.69	1.30	1.42
5	B	507	SIA	C3-C4	-2.53	1.48	1.52
5	B	507	SIA	C6-C5	-2.36	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	503	BMA	O6-C6	2.05	1.51	1.42
5	B	507	SIA	C11-C10	2.07	1.54	1.50
5	B	504	MAN	O5-C1	2.58	1.48	1.43
5	B	507	SIA	C5-N5	2.69	1.50	1.45
3	A	502	NAG	C7-N2	2.92	1.45	1.34
4	C	508	NAG	C7-N2	2.96	1.45	1.34
3	A	505	NAG	C7-N2	2.96	1.45	1.34
8	D	502	NAG	C7-N2	2.96	1.45	1.34
6	C	504	MAN	O5-C1	3.04	1.48	1.43
4	C	507	MAN	O5-C1	3.05	1.48	1.43
4	A	506	MAN	O5-C1	3.05	1.48	1.43
4	B	508	MAN	O5-C1	3.07	1.48	1.43
4	D	504	MAN	O5-C1	3.09	1.48	1.43
9	D	506	MAN	O5-C1	3.09	1.48	1.43
6	C	506	GAL	O5-C1	3.18	1.49	1.43
5	B	506	GAL	O5-C1	3.20	1.49	1.43
5	B	507	SIA	C10-N5	3.24	1.46	1.34
4	C	508	NAG	O5-C1	3.69	1.49	1.43
3	A	502	NAG	O5-C1	3.70	1.49	1.43
3	A	505	NAG	O5-C1	3.74	1.50	1.43
8	D	502	NAG	O5-C1	3.74	1.50	1.43
5	B	507	SIA	O6-C2	3.79	1.54	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	503	BMA	C6-C5-C4	-7.50	94.50	113.02
5	B	504	MAN	O5-C1-C2	-5.87	101.33	110.86
5	B	507	SIA	C7-C6-C5	-3.72	108.70	114.32
3	A	503	BMA	O3-C3-C4	-3.41	102.66	110.34
3	A	503	BMA	O6-C6-C5	-2.79	102.10	111.33
5	B	502	NAG	O7-C7-C8	-2.58	117.32	122.06
8	D	501	NAG	O6-C6-C5	-2.50	103.06	111.33
5	B	501	NAG	O6-C6-C5	-2.50	103.08	111.33
3	A	505	NAG	C2-N2-C7	-2.48	119.85	123.04
4	C	508	NAG	C2-N2-C7	-2.48	119.86	123.04
8	D	502	NAG	C2-N2-C7	-2.46	119.88	123.04
3	A	502	NAG	C2-N2-C7	-2.44	119.90	123.04
8	D	503	BMA	O3-C3-C4	-2.27	105.23	110.34
5	B	503	BMA	O3-C3-C4	-2.25	105.27	110.34
6	C	503	BMA	O3-C3-C4	-2.24	105.30	110.34
8	D	502	NAG	C8-C7-N2	2.01	119.95	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	NAG	C8-C7-N2	2.01	119.95	116.11
3	A	502	NAG	C8-C7-N2	2.02	119.97	116.11
5	B	501	NAG	C8-C7-N2	2.02	119.97	116.11
4	C	508	NAG	C8-C7-N2	2.03	120.00	116.11
5	B	507	SIA	C11-C10-N5	2.03	120.00	116.11
9	D	508	GAL	C1-O5-C5	2.14	114.97	112.25
5	B	502	NAG	O5-C5-C6	2.21	112.13	107.35
4	C	507	MAN	C1-C2-C3	2.22	112.16	109.54
4	B	508	MAN	C1-C2-C3	2.22	112.16	109.54
4	D	504	MAN	C1-C2-C3	2.24	112.19	109.54
6	C	504	MAN	C1-C2-C3	2.25	112.20	109.54
4	A	506	MAN	C1-C2-C3	2.25	112.20	109.54
9	D	506	MAN	C1-C2-C3	2.27	112.23	109.54
4	D	505	NAG	C8-C7-N2	2.32	120.56	116.11
5	B	506	GAL	C1-C2-C3	2.34	112.31	109.54
4	B	509	NAG	C8-C7-N2	2.34	120.58	116.11
6	C	506	GAL	C1-C2-C3	2.36	112.33	109.54
5	B	501	NAG	C1-O5-C5	2.55	115.48	112.25
8	D	501	NAG	C1-O5-C5	2.56	115.50	112.25
8	D	503	BMA	C3-C4-C5	2.66	114.83	110.20
5	B	503	BMA	C3-C4-C5	2.66	114.84	110.20
5	B	502	NAG	C4-C3-C2	2.69	115.41	111.23
6	C	503	BMA	C3-C4-C5	2.70	114.91	110.20
5	B	507	SIA	O6-C6-C5	2.74	112.97	108.48
3	A	503	BMA	C1-O5-C5	3.11	116.19	112.25
4	A	507	NAG	C1-O5-C5	3.29	116.42	112.25
5	B	503	BMA	C1-O5-C5	3.49	116.68	112.25
8	D	503	BMA	C1-O5-C5	3.49	116.68	112.25
6	C	503	BMA	C1-O5-C5	3.51	116.70	112.25
6	C	503	BMA	O5-C5-C6	3.70	115.35	107.35
5	B	503	BMA	O6-C6-C5	3.91	124.25	111.33
3	A	504	MAN	C1-O5-C5	4.81	118.36	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	D	501	NAG	C1
9	D	506	MAN	C1
6	C	504	MAN	C1

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	11	0
3	A	503	BMA	3	0
4	A	506	MAN	3	0
5	B	501	NAG	2	0
5	B	502	NAG	2	0
5	B	503	BMA	5	0
5	B	504	MAN	1	0
5	B	506	GAL	2	0
4	B	508	MAN	8	0
6	C	503	BMA	8	0
6	C	504	MAN	1	0
6	C	505	NAG	2	0
6	C	506	GAL	6	0
4	C	507	MAN	6	0
8	D	503	BMA	6	0
4	D	504	MAN	7	0
9	D	506	MAN	1	0
9	D	507	NAG	3	0
9	D	508	GAL	1	0

5.6 Ligand geometry

4 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	1,3	14,14,15	1.56	2 (14%)	15,19,21	1.14	2 (13%)
2	NAG	C	501	1,2	14,14,15	1.55	2 (14%)	15,19,21	1.14	2 (13%)
2	NAG	C	502	2,6	14,14,15	0.72	0	15,19,21	1.35	3 (20%)
7	SIA	C	509	6	16,20,21	1.93	7 (43%)	18,28,31	1.46	3 (16%)

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	1,3	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	2,6	-	0/6/23/26	0/1/1/1
7	SIA	C	509	6	-	0/14/34/38	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	509	SIA	C3-C4	-2.49	1.48	1.52
7	C	509	SIA	C6-C5	-2.40	1.49	1.53
7	C	509	SIA	O8-C8	-2.01	1.38	1.43
7	C	509	SIA	C11-C10	2.04	1.54	1.50
7	C	509	SIA	C5-N5	2.73	1.50	1.45
2	C	501	NAG	C7-N2	2.94	1.45	1.34
2	A	501	NAG	C7-N2	2.96	1.45	1.34
7	C	509	SIA	C10-N5	3.25	1.46	1.34
2	A	501	NAG	O5-C1	3.73	1.50	1.43
2	C	501	NAG	O5-C1	3.73	1.50	1.43
7	C	509	SIA	O6-C2	3.78	1.54	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	509	SIA	C7-C6-C5	-3.72	108.69	114.32
2	C	502	NAG	O7-C7-C8	-2.58	117.33	122.06
2	C	501	NAG	C2-N2-C7	-2.47	119.87	123.04
2	A	501	NAG	C2-N2-C7	-2.46	119.88	123.04
2	A	501	NAG	C8-C7-N2	2.01	119.96	116.11
7	C	509	SIA	C11-C10-N5	2.03	120.00	116.11
2	C	501	NAG	C8-C7-N2	2.04	120.01	116.11
2	C	502	NAG	O5-C5-C6	2.23	112.18	107.35
2	C	502	NAG	C4-C3-C2	2.65	115.35	111.23
7	C	509	SIA	O6-C6-C5	2.71	112.93	108.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	2	0
2	C	501	NAG	7	0
2	C	502	NAG	8	0
7	C	509	SIA	7	14

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	208/221 (94%)	0.29	8 (3%)	44	18	22, 70, 149, 268	0
1	B	206/221 (93%)	0.03	1 (0%)	91	76	15, 54, 111, 169	1 (0%)
1	C	199/221 (90%)	0.43	22 (11%)	7	3	14, 70, 174, 262	0
1	D	195/221 (88%)	0.31	14 (7%)	18	7	16, 53, 156, 215	0
All	All	808/884 (91%)	0.26	45 (5%)	28	11	14, 62, 151, 268	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	239	SER	6.9
1	C	271	PRO	6.5
1	C	285	HIS	5.7
1	C	266	VAL	5.5
1	D	262	VAL	5.3
1	D	263	VAL	4.6
1	C	273	VAL	4.5
1	D	239	SER	4.4
1	C	302	VAL	4.3
1	D	276	ASN	3.7
1	B	295	GLN	3.6
1	D	240	VAL	3.6
1	D	241	PHE	3.5
1	C	300	TYR	3.4
1	C	264	VAL	3.4
1	C	240	VAL	3.3
1	D	275	PHE	3.3
1	C	265	ASP	3.3
1	A	298	SER	3.2
1	D	304	SER	3.2
1	D	323	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	SER	2.9
1	D	316	GLY	2.9
1	A	265	ASP	2.9
1	C	268	HIS	2.7
1	C	299	THR	2.6
1	A	253	ILE	2.6
1	D	273	VAL	2.6
1	C	323	VAL	2.6
1	A	309	LEU	2.5
1	C	333	GLU	2.4
1	D	301	ARG	2.3
1	C	296	TYR	2.3
1	A	308	VAL	2.2
1	A	422	VAL	2.2
1	C	267	SER	2.2
1	C	262	VAL	2.2
1	C	306	LEU	2.2
1	C	325	ASN	2.2
1	C	238	PRO	2.1
1	C	383	SER	2.1
1	D	294	GLU	2.1
1	C	263	VAL	2.1
1	D	306	LEU	2.1
1	A	251	LEU	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. 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(\AA^2)	Q<0.9
9	GAL	D	508	11/12	0.38	0.54	5.15	85,85,85,85	0
5	GAL	B	506	11/12	0.78	0.31	1.83	27,32,41,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GAL	C	506	11/12	0.60	0.30	0.98	64,69,78,95	0
5	NAG	B	502	14/15	0.87	0.25	-0.26	26,36,43,43	0
4	NAG	C	508	14/15	0.58	0.38	-	80,90,102,104	0
3	NAG	A	505	14/15	0.71	0.33	-	105,111,118,120	0
5	NAG	B	501	14/15	0.80	0.29	-	46,52,58,60	0
6	NAG	C	505	14/15	0.77	0.27	-	47,53,58,59	0
5	SIA	B	507	20/21	0.71	0.37	-	122,131,136,136	0
4	NAG	A	507	14/15	0.59	0.40	-	99,105,109,110	0
4	MAN	D	504	11/12	0.74	0.31	-	127,136,139,155	0
4	NAG	B	509	14/15	0.68	0.28	-	88,98,110,112	0
5	BMA	B	503	11/12	0.66	0.34	-	67,71,75,77	0
6	BMA	C	503	11/12	0.76	0.27	-	101,105,110,111	0
8	NAG	D	501	14/15	0.57	0.35	-	174,180,186,188	0
9	MAN	D	506	11/12	0.78	0.38	-	114,114,114,114	0
8	BMA	D	503	11/12	0.55	0.39	-	74,79,83,84	0
3	NAG	A	502	14/15	0.82	0.38	-	81,85,89,91	0
8	NAG	D	502	14/15	0.80	0.25	-	96,106,112,113	0
4	MAN	C	507	11/12	0.72	0.30	-	97,106,109,125	0
9	NAG	D	507	14/15	0.69	0.39	-	59,65,70,71	0
4	MAN	A	506	11/12	0.66	0.27	-	133,137,143,151	0
4	NAG	D	505	14/15	0.56	0.35	-	108,118,131,132	0
6	MAN	C	504	11/12	0.55	0.27	-	88,91,98,108	0
3	MAN	A	504	11/12	0.67	0.35	-	88,89,94,99	0
5	NAG	B	505	14/15	0.84	0.32	-	72,78,83,84	0
4	MAN	B	508	11/12	0.77	0.35	-	87,97,100,115	0
5	MAN	B	504	11/12	0.79	0.20	-	41,44,51,61	0
3	BMA	A	503	11/12	0.82	0.16	-	74,76,78,80	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. 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(\AA^2)	Q<0.9
7	SIA	C	509	20/21	0.71	0.35	0.29	80,89,93,93	0
2	NAG	A	501	14/15	0.70	0.34	-0.18	78,79,81,83	0
2	NAG	C	502	14/15	0.72	0.38	-	96,106,113,113	0
2	NAG	C	501	14/15	0.67	0.41	-	101,107,113,115	0

6.5 Other polymers

There are no such residues in this entry.