



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:03 PM GMT

PDB ID : 4GZX  
Title : N2 neuraminidase D151G mutant of A/Tanzania/205/2010 H3N2 in complex with human sialic acid receptor  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2012-09-06  
Resolution : 2.45 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](mailto: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.

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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

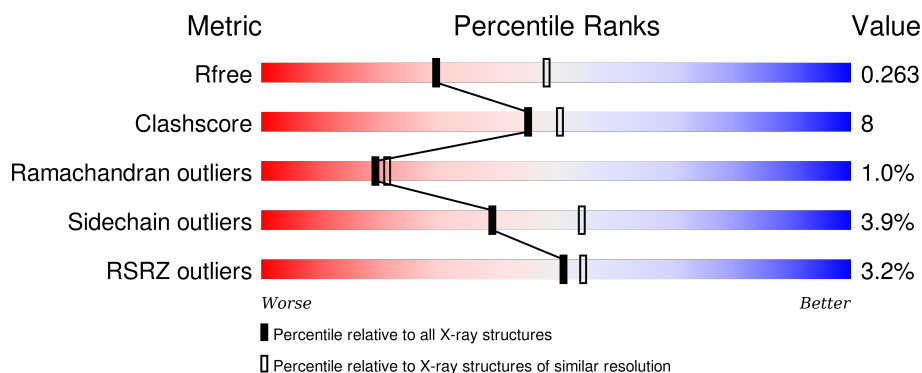
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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  $\geq 3$ , 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	393	<div> <div>3%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
1	B	393	<div> <div>4%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	393	<div> <div>4%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	D	393	<div> <div>3%</div> <div>81%</div> <div>17%</div> <div>..</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
4	NAG	B	810	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13064 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 neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	B	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	C	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	D	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			32	17	1	14		
2	B	2	Total	C	N	O	0	0
			32	17	1	14		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	B	5	Total	C	N	O	0	0
			61	34	2	25		
3	C	5	Total	C	N	O	0	0
			61	34	2	25		
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

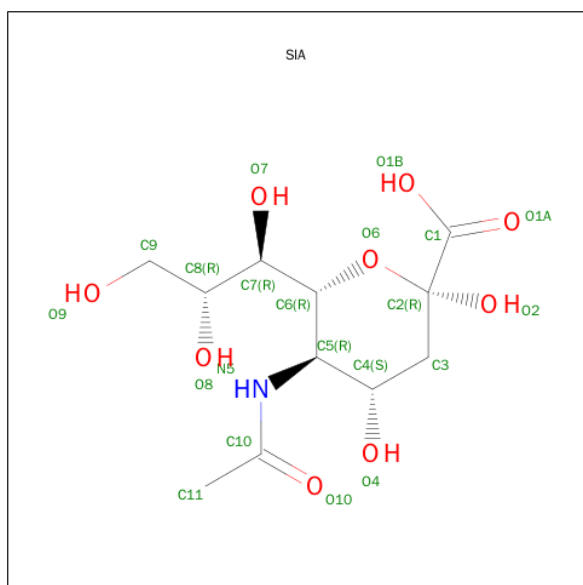
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			21	11	1	9		
6	D	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	2	Total	C	N	O	0	0
			24	14	1	9		

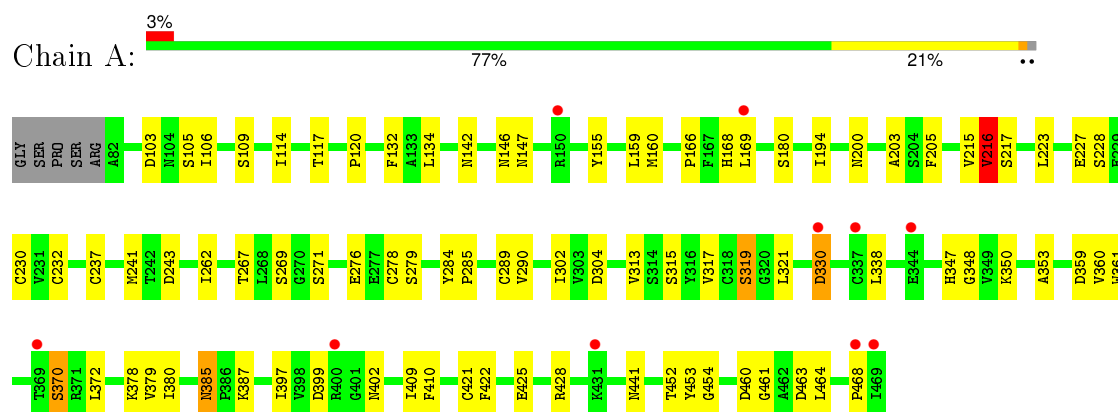
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	147	Total 147	O 147	0	0
9	B	139	Total 139	O 139	0	0
9	C	99	Total 99	O 99	0	0
9	D	130	Total 130	O 130	0	0

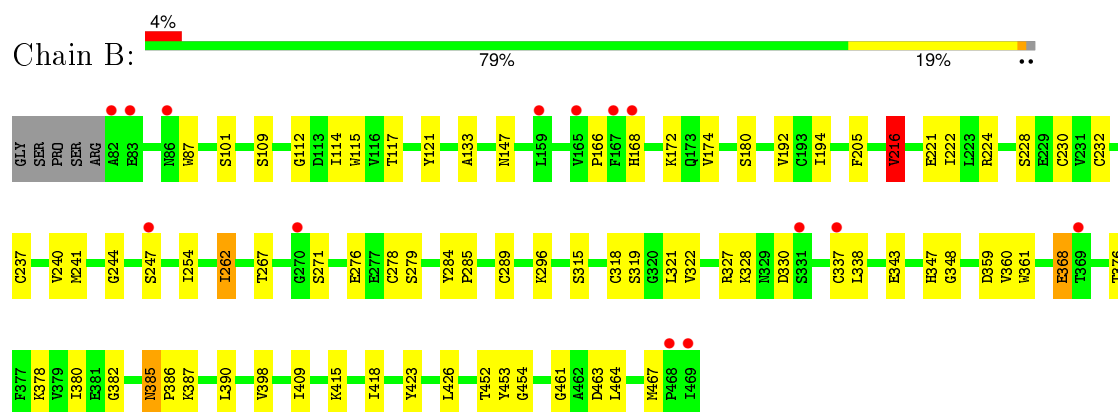
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

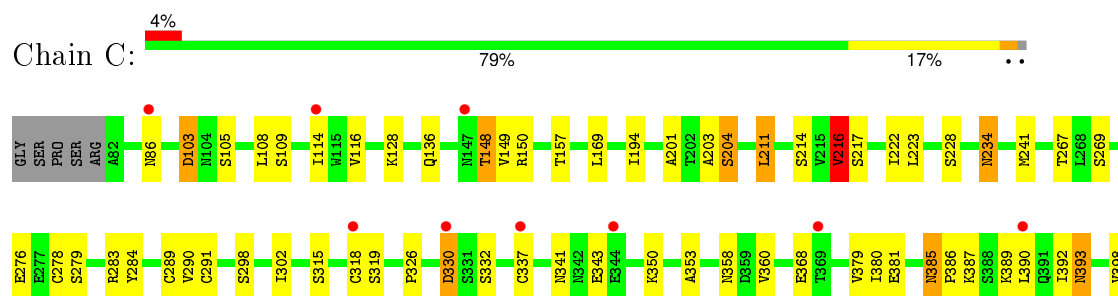
#### • Molecule 1: neuraminidase



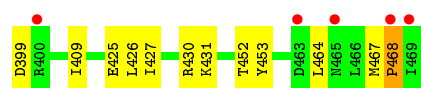
#### • Molecule 1: neuraminidase



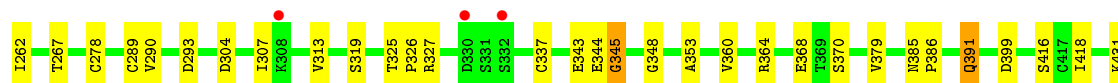
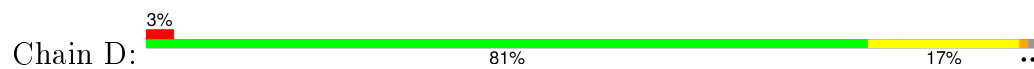
#### • Molecule 1: neuraminidase







● Molecule 1: neuraminidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.59Å 110.18Å 110.04Å 90.00° 97.45° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 44.04 – 2.45	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.45) 84.3 (44.04-2.45)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.271 0.211 , 0.263	Depositor DCC
$R_{free}$ test set	2997 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	1.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 59112 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, NAG, CA, SIA, GAL, FUC, FUL, 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	0.54	0/3065	0.69	1/4156 (0.0%)
1	B	0.53	0/3065	0.67	1/4156 (0.0%)
1	C	0.53	0/3065	0.67	1/4156 (0.0%)
1	D	0.51	0/3065	0.67	1/4156 (0.0%)
All	All	0.53	0/12260	0.67	4/16624 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	VAL	CB-CA-C	-6.12	99.77	111.40
1	C	216	VAL	CB-CA-C	-5.94	100.11	111.40
1	B	216	VAL	CB-CA-C	-5.12	101.66	111.40
1	A	216	VAL	CB-CA-C	-5.04	101.83	111.40

There are no chirality outliers.

There are no planarity outliers.

### 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	2998	0	2855	59	0
1	B	2998	0	2855	57	0
1	C	2998	0	2855	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2998	0	2855	42	0
2	A	32	0	28	0	0
2	B	32	0	28	0	0
3	A	61	0	52	0	0
3	B	61	0	52	1	0
3	C	61	0	52	1	0
3	D	61	0	52	1	0
4	A	42	0	39	2	0
4	B	42	0	39	3	0
4	C	28	0	26	0	0
4	D	28	0	26	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	21	0	18	0	0
6	D	21	0	18	0	0
7	C	38	0	34	1	0
8	D	24	0	22	1	0
9	A	147	0	0	2	0
9	B	139	0	0	1	0
9	C	99	0	0	2	0
9	D	130	0	0	0	0
All	All	13064	0	11906	190	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 8.

All (190) 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:C:109:SER:HB3	1:C:114:ILE:HB	1.54	0.90
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.59	0.83
1:A:216:VAL:HG22	1:B:452:THR:HB	1.58	0.83
1:A:271:SER:HB3	1:A:338:LEU:O	1.86	0.75
1:C:216:VAL:HG22	1:D:452:THR:HB	1.68	0.74
1:B:385:ASN:HD22	1:B:387:LYS:H	1.35	0.74
1:A:452:THR:HB	1:D:216:VAL:HG22	1.70	0.73
1:C:279:SER:HB3	1:C:409:ILE:HG22	1.71	0.72
1:A:279:SER:HB3	1:A:409:ILE:HG22	1.70	0.70
1:B:216:VAL:CG2	1:C:452:THR:HB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:VAL:HG12	1:C:379:VAL:HB	1.72	0.70
1:A:385:ASN:ND2	1:A:387:LYS:H	1.91	0.69
1:A:146:ASN:O	1:A:147:ASN:HB2	1.93	0.68
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.77	0.67
1:A:385:ASN:HD21	1:A:387:LYS:HB2	1.61	0.66
1:A:330:ASP:N	1:A:330:ASP:OD1	2.28	0.66
1:A:120:PRO:HD3	1:A:425:GLU:OE2	1.96	0.66
1:A:452:THR:CB	1:D:216:VAL:HG22	2.27	0.65
1:C:228:SER:HB3	1:C:350:LYS:CE	2.27	0.64
1:B:147:ASN:HD21	4:B:809:NAG:H62	1.63	0.63
1:C:385:ASN:HD22	1:C:385:ASN:C	2.01	0.63
1:B:385:ASN:ND2	1:B:387:LYS:H	1.97	0.63
1:A:109:SER:HB3	1:A:114:ILE:HB	1.80	0.63
1:B:109:SER:HB3	1:B:114:ILE:HB	1.80	0.62
1:B:216:VAL:HG23	1:C:452:THR:OG1	2.00	0.62
1:B:278:CYS:HB3	1:B:289:CYS:HB3	1.81	0.62
1:B:328:LYS:HD2	1:B:343:GLU:OE1	2.00	0.60
1:D:446:PHE:HZ	1:D:458:TRP:CE3	2.18	0.60
1:A:216:VAL:CG2	1:B:452:THR:HB	2.30	0.60
1:A:454:GLY:HA3	1:D:200:ASN:O	2.02	0.59
1:A:453:TYR:C	1:D:216:VAL:HG13	2.23	0.59
1:B:87:TRP:HE3	1:B:418:ILE:HD12	1.66	0.59
1:A:461:GLY:HA3	1:D:155:TYR:CE1	2.39	0.58
1:A:216:VAL:HG13	1:B:453:TYR:C	2.24	0.57
1:C:216:VAL:HG13	1:D:453:TYR:O	2.04	0.57
1:C:204:SER:HB3	1:C:211:LEU:HD11	1.87	0.57
1:A:166:PRO:O	1:A:168:HIS:HD2	1.87	0.57
1:B:194:ILE:HD11	1:B:241:MET:CE	2.36	0.56
1:C:194:ILE:HD11	1:C:241:MET:CE	2.36	0.56
1:A:223:LEU:HD11	1:A:241:MET:HE2	1.87	0.55
1:C:216:VAL:HG22	1:D:452:THR:CB	2.35	0.55
1:A:217:SER:OG	1:A:243:ASP:OD2	2.20	0.55
1:C:216:VAL:HG13	1:D:453:TYR:C	2.27	0.55
1:A:284:TYR:CD1	1:A:285:PRO:HA	2.42	0.54
3:C:804:BMA:H4	1:D:391:GLN:O	2.08	0.54
1:B:360:VAL:HG12	1:B:382:GLY:HA3	1.89	0.54
1:C:278:CYS:HB3	1:C:289:CYS:HB3	1.90	0.53
1:B:380:ILE:HD12	1:B:390:LEU:HG	1.90	0.53
1:B:228:SER:HB3	1:B:423:TYR:OH	2.08	0.53
1:B:216:VAL:HG23	1:C:452:THR:CB	2.38	0.53
1:A:168:HIS:HB2	9:A:933:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:PRO:HA	1:D:368:GLU:O	2.08	0.53
1:A:205:PHE:CE1	1:A:262:ILE:HD11	2.44	0.53
1:A:271:SER:HB2	1:A:315:SER:HA	1.92	0.52
1:C:194:ILE:HG21	1:C:223:LEU:O	2.09	0.52
1:A:302:ILE:HD11	1:A:317:VAL:HA	1.91	0.52
1:D:278:CYS:HB3	1:D:289:CYS:HB3	1.91	0.52
1:B:216:VAL:HG22	1:C:453:TYR:N	2.25	0.52
1:A:428:ARG:NH1	1:A:460:ASP:OD2	2.41	0.51
1:A:169:LEU:HD11	1:B:112:GLY:HA3	1.92	0.51
1:C:398:VAL:HG21	1:C:426:LEU:HD21	1.92	0.51
1:B:216:VAL:HG23	1:C:452:THR:HB	1.92	0.51
1:C:194:ILE:HD11	1:C:241:MET:HE3	1.92	0.51
1:B:347:HIS:CG	1:B:348:GLY:H	2.30	0.50
1:A:360:VAL:HG12	1:A:379:VAL:HB	1.94	0.49
4:A:810:NAG:H81	9:A:1040:HOH:O	2.13	0.49
1:C:330:ASP:O	1:C:389:LYS:NZ	2.27	0.49
1:C:150:ARG:HH12	7:C:809:FUC:H63	1.76	0.49
1:D:107:ARG:HD2	1:D:461:GLY:HA3	1.94	0.48
1:A:428:ARG:NH2	1:A:464:LEU:HG	2.28	0.48
1:B:361:TRP:CE2	1:B:378:LYS:HD3	2.49	0.48
1:A:200:ASN:O	1:B:454:GLY:HA3	2.13	0.48
1:C:86:ASN:ND2	1:C:234:ASN:OD1	2.42	0.48
1:B:267:THR:HG22	9:B:982:HOH:O	2.13	0.48
1:C:298:SER:OG	1:C:341:ASN:ND2	2.45	0.48
1:B:117:THR:HB	1:B:133:ALA:HB1	1.96	0.48
1:B:194:ILE:HD11	1:B:241:MET:HE3	1.95	0.48
1:C:430:ARG:HB3	1:C:431:LYS:HA	1.96	0.48
1:C:385:ASN:ND2	1:C:387:LYS:H	2.12	0.48
1:B:232:CYS:HA	1:B:237:CYS:HA	1.96	0.48
1:C:116:VAL:HG11	1:C:148:THR:HG21	1.96	0.48
1:A:304:ASP:HB2	1:A:313:VAL:HG22	1.95	0.48
1:C:318:CYS:O	1:C:386:PRO:HA	2.14	0.47
1:A:452:THR:OG1	1:D:216:VAL:HG22	2.14	0.47
1:B:121:TYR:CG	1:B:228:SER:HA	2.49	0.47
1:D:158:LEU:O	1:D:174:VAL:HG22	2.14	0.47
1:A:168:HIS:CD2	1:A:168:HIS:H	2.32	0.47
1:B:271:SER:HB2	1:B:338:LEU:O	2.14	0.47
1:C:276:GLU:O	1:C:291:CYS:HB3	2.14	0.47
1:B:318:CYS:O	1:B:386:PRO:HA	2.15	0.47
1:D:87:TRP:HE3	1:D:418:ILE:HD12	1.80	0.47
1:A:385:ASN:HD22	1:A:385:ASN:C	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG21	1:C:353:ALA:HB3	1.97	0.46
1:B:87:TRP:CE3	1:B:418:ILE:HD12	2.49	0.46
1:A:132:PHE:CE2	1:A:160:MET:HG3	2.49	0.46
1:C:203:ALA:O	1:C:214:SER:HA	2.15	0.46
1:B:205:PHE:CE1	1:B:262:ILE:HD11	2.50	0.46
1:D:343:GLU:C	1:D:345:GLY:H	2.18	0.46
1:B:398:VAL:HG21	1:B:426:LEU:CD2	2.46	0.46
1:C:380:ILE:HD12	1:C:390:LEU:HD23	1.97	0.46
1:A:410:PHE:CZ	1:A:421:CYS:HB2	2.50	0.46
1:B:385:ASN:C	1:B:385:ASN:HD22	2.19	0.46
1:C:467:MET:HB3	1:C:468:PRO:HD2	1.98	0.46
1:A:397:ILE:HG13	1:A:422:PHE:HZ	1.81	0.46
1:D:102:LYS:NZ	1:D:104:ASN:OD1	2.47	0.46
1:B:224:ARG:NE	1:B:276:GLU:OE1	2.39	0.46
1:A:194:ILE:HD11	1:A:241:MET:CE	2.46	0.45
1:B:361:TRP:CZ2	1:B:378:LYS:HD3	2.52	0.45
1:B:296:LYS:HB2	1:B:296:LYS:HE3	1.79	0.45
1:A:399:ASP:OD1	1:A:402:ASN:OD1	2.35	0.45
1:B:240:VAL:HG22	1:B:254:ILE:HG13	1.97	0.45
1:C:201:ALA:H	1:C:217:SER:HB2	1.81	0.45
1:B:147:ASN:HD21	4:B:809:NAG:C6	2.29	0.45
1:B:284:TYR:CD1	1:B:285:PRO:HA	2.52	0.45
1:B:115:TRP:CH2	1:C:108:LEU:HD21	2.52	0.44
1:D:205:PHE:CE1	1:D:262:ILE:HD11	2.52	0.44
1:B:398:VAL:HG21	1:B:426:LEU:HD21	1.98	0.44
1:C:358:ASN:ND2	9:C:989:HOH:O	2.50	0.44
1:C:392:ILE:O	1:C:393:ASN:HB2	2.17	0.44
1:A:453:TYR:HA	1:D:202:THR:HG23	1.99	0.44
1:C:136:GLN:HE21	1:C:136:GLN:HA	1.82	0.44
1:D:213:ASP:OD1	1:D:214:SER:N	2.49	0.44
1:A:453:TYR:O	1:D:216:VAL:HG13	2.18	0.44
1:C:315:SER:HB2	1:C:337:CYS:O	2.18	0.44
1:B:359:ASP:OD1	1:B:380:ILE:HA	2.18	0.43
1:D:337:CYS:SG	1:D:386:PRO:HD3	2.58	0.43
1:B:464:LEU:HA	1:B:467:MET:HG2	2.00	0.43
1:C:464:LEU:HA	1:C:467:MET:HG3	2.01	0.43
1:A:228:SER:HB3	1:A:350:LYS:HE2	2.01	0.43
1:C:326:PRO:HA	1:C:368:GLU:O	2.18	0.43
1:C:385:ASN:HD22	1:C:387:LYS:H	1.65	0.43
1:B:279:SER:HB3	1:B:409:ILE:HG22	2.00	0.43
1:B:315:SER:HB2	1:B:337:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:CE2	1:A:378:LYS:HD3	2.53	0.43
1:D:132:PHE:CE1	1:D:160:MET:HG3	2.54	0.43
1:D:431:LYS:HE2	1:D:431:LYS:HB3	1.85	0.43
1:D:103:ASP:OD2	1:D:105:SER:HB2	2.18	0.43
1:B:321:LEU:HD22	1:B:330:ASP:OD1	2.19	0.43
1:B:115:TRP:CZ2	1:C:108:LEU:HD21	2.54	0.43
1:D:147:ASN:HD21	8:D:808:NAG:H62	1.82	0.43
1:C:103:ASP:OD2	1:C:105:SER:HB2	2.19	0.43
1:A:359:ASP:OD1	1:A:380:ILE:HA	2.19	0.42
1:C:380:ILE:O	1:C:381:GLU:HB2	2.19	0.42
1:B:180:SER:HA	1:B:192:VAL:O	2.20	0.42
1:C:149:VAL:HG21	1:C:431:LYS:HG3	2.01	0.42
1:A:232:CYS:HA	1:A:237:CYS:HA	2.00	0.42
1:D:290:VAL:HG21	1:D:353:ALA:HB3	2.00	0.42
1:A:147:ASN:HD21	4:A:809:NAG:C6	2.33	0.42
1:A:321:LEU:HD12	1:A:379:VAL:HG22	2.02	0.42
1:D:125:ASP:HB2	1:D:126:PRO:CD	2.50	0.42
1:C:136:GLN:NE2	1:C:136:GLN:HA	2.35	0.42
1:D:325:THR:O	1:D:348:GLY:HA2	2.20	0.42
1:A:347:HIS:CG	1:A:348:GLY:H	2.38	0.42
1:B:192:VAL:HG22	1:B:205:PHE:CD2	2.55	0.42
1:A:453:TYR:O	3:D:802:NAG:H62	2.20	0.41
1:C:360:VAL:CG1	1:C:379:VAL:HB	2.45	0.41
1:C:341:ASN:ND2	1:C:343:GLU:HB2	2.35	0.41
1:A:106:ILE:HD11	1:A:441:ASN:C	2.41	0.41
1:B:166:PRO:O	1:B:168:HIS:HD2	2.03	0.41
1:A:155:TYR:CZ	1:B:461:GLY:HA3	2.55	0.41
1:C:385:ASN:ND2	1:C:385:ASN:C	2.70	0.41
1:D:343:GLU:O	1:D:345:GLY:N	2.54	0.41
1:B:322:VAL:HG23	1:B:327:ARG:HD2	2.03	0.41
1:C:289:CYS:O	1:C:302:ILE:HA	2.20	0.41
1:A:370:SER:HB3	1:A:372:LEU:HD23	2.02	0.41
1:D:360:VAL:HG12	1:D:379:VAL:HB	2.02	0.41
1:B:221:GLU:HB3	1:B:244:GLY:HA2	2.03	0.41
3:B:804:NAG:H3	1:C:393:ASN:HA	2.03	0.41
1:A:452:THR:O	1:D:214:SER:OG	2.38	0.41
1:A:117:THR:HA	1:A:134:LEU:O	2.21	0.41
1:B:368:GLU:OE1	4:B:810:NAG:H82	2.21	0.41
1:C:128:LYS:HE3	9:C:907:HOH:O	2.20	0.41
1:D:304:ASP:HB2	1:D:313:VAL:HG23	2.03	0.41
1:C:425:GLU:HG2	1:C:427:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ASN:HA	1:B:386:PRO:HD2	1.89	0.41
1:A:194:ILE:HG12	1:A:203:ALA:HB2	2.03	0.41
1:D:217:SER:OG	1:D:243:ASP:OD2	2.26	0.41
1:C:169:LEU:HD23	1:C:169:LEU:HA	1.71	0.41
1:D:120:PRO:HA	1:D:132:PHE:O	2.20	0.41
1:C:283:ARG:O	1:C:284:TYR:C	2.59	0.41
1:D:385:ASN:HA	1:D:386:PRO:HD2	1.98	0.40
1:A:290:VAL:HG21	1:A:353:ALA:HB3	2.03	0.40
1:A:385:ASN:ND2	1:A:385:ASN:C	2.74	0.40
1:B:194:ILE:HD11	1:B:241:MET:HE2	2.02	0.40
1:D:119:GLU:N	1:D:120:PRO:CD	2.84	0.40
1:D:327:ARG:CZ	1:D:364:ARG:HD2	2.52	0.40
1:A:132:PHE:HA	1:A:159:LEU:O	2.22	0.40
1:D:212:VAL:HB	1:D:260:GLY:HA3	2.03	0.40
1:A:194:ILE:HD11	1:A:241:MET:HE3	2.04	0.40
1:D:293:ASP:C	1:D:293:ASP:OD1	2.59	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	386/393 (98%)	354 (92%)	29 (8%)	3 (1%)	24	28
1	B	386/393 (98%)	358 (93%)	25 (6%)	3 (1%)	24	28
1	C	386/393 (98%)	360 (93%)	22 (6%)	4 (1%)	19	21
1	D	386/393 (98%)	356 (92%)	25 (6%)	5 (1%)	15	15
All	All	1544/1572 (98%)	1428 (92%)	101 (6%)	15 (1%)	19	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	393	ASN
1	D	319	SER
1	D	345	GLY
1	A	468	PRO
1	D	344	GLU
1	A	319	SER
1	B	319	SER
1	C	319	SER
1	D	468	PRO
1	A	142	ASN
1	C	222	ILE
1	D	247	SER
1	B	262	ILE
1	C	468	PRO
1	B	222	ILE

### 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	337/341 (99%)	322 (96%)	15 (4%)	34	47
1	B	337/341 (99%)	326 (97%)	11 (3%)	45	61
1	C	337/341 (99%)	324 (96%)	13 (4%)	39	54
1	D	337/341 (99%)	324 (96%)	13 (4%)	39	54
All	All	1348/1364 (99%)	1296 (96%)	52 (4%)	39	54

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	105	SER
1	A	180	SER
1	A	215	VAL
1	A	216	VAL
1	A	227	GLU
1	A	230	CYS

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Mol	Chain	Res	Type
1	A	267	THR
1	A	269	SER
1	A	276	GLU
1	A	319	SER
1	A	330	ASP
1	A	370	SER
1	A	385	ASN
1	A	463	ASP
1	B	101	SER
1	B	172	LYS
1	B	174	VAL
1	B	216	VAL
1	B	230	CYS
1	B	247	SER
1	B	368	GLU
1	B	376	THR
1	B	385	ASN
1	B	415	LYS
1	B	463	ASP
1	C	103	ASP
1	C	148	THR
1	C	157	THR
1	C	204	SER
1	C	211	LEU
1	C	216	VAL
1	C	234	ASN
1	C	267	THR
1	C	269	SER
1	C	330	ASP
1	C	332	SER
1	C	385	ASN
1	C	399	ASP
1	D	139	THR
1	D	140	LEU
1	D	180	SER
1	D	214	SER
1	D	216	VAL
1	D	261	LYS
1	D	267	THR
1	D	307	ILE
1	D	370	SER
1	D	391	GLN

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Mol	Chain	Res	Type
1	D	399	ASP
1	D	416	SER
1	D	443	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	147	ASN
1	A	168	HIS
1	A	358	ASN
1	A	385	ASN
1	A	393	ASN
1	A	402	ASN
1	B	136	GLN
1	B	147	ASN
1	B	168	HIS
1	B	385	ASN
1	B	393	ASN
1	C	136	GLN
1	C	358	ASN
1	C	385	ASN
1	D	136	GLN
1	D	147	ASN
1	D	168	HIS
1	D	385	ASN
1	D	465	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

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	$\# Z  > 2$
2	SIA	A	801	2	16,20,21	0.70	1 (6%)	18,28,31	1.21	2 (11%)
2	GAL	A	802	2	12,12,12	0.65	0	17,17,17	0.84	1 (5%)
3	NAG	A	803	1,3	14,14,15	0.62	0	15,19,21	1.47	2 (13%)
3	NAG	A	804	3	14,14,15	0.44	0	15,19,21	1.53	3 (20%)
3	BMA	A	805	3	11,11,12	0.62	0	14,15,17	1.01	1 (7%)
3	MAN	A	806	3	11,11,12	0.69	0	14,15,17	1.37	2 (14%)
3	MAN	A	807	3	11,11,12	0.68	0	14,15,17	2.33	3 (21%)
2	SIA	B	801	2	16,20,21	0.52	0	18,28,31	0.93	2 (11%)
2	GAL	B	802	2	12,12,12	0.67	0	17,17,17	1.90	4 (23%)
3	NAG	B	803	1,3	14,14,15	0.57	0	15,19,21	0.83	0
3	NAG	B	804	3	14,14,15	0.56	0	15,19,21	1.49	3 (20%)
3	BMA	B	805	3	11,11,12	0.82	0	14,15,17	1.01	0
3	MAN	B	806	3	11,11,12	0.59	0	14,15,17	1.87	2 (14%)
3	MAN	B	807	3	11,11,12	0.48	0	14,15,17	2.53	3 (21%)
3	NAG	C	802	1,3	14,14,15	0.61	0	15,19,21	1.16	0
3	NAG	C	803	3	14,14,15	0.45	0	15,19,21	1.55	3 (20%)
3	BMA	C	804	3	11,11,12	0.69	0	14,15,17	1.00	0
3	MAN	C	805	3	11,11,12	0.65	0	14,15,17	1.52	3 (21%)
3	MAN	C	806	3	11,11,12	0.67	0	14,15,17	3.02	4 (28%)
7	NAG	C	807	1,7	14,14,15	0.63	0	15,19,21	1.41	2 (13%)
7	NAG	C	808	7	14,14,15	0.68	0	15,19,21	1.14	1 (6%)
7	FUC	C	809	7	10,10,11	0.58	0	14,14,16	1.15	1 (7%)
3	NAG	D	802	1,3	14,14,15	0.65	0	15,19,21	0.96	0
3	NAG	D	803	3	14,14,15	0.37	0	15,19,21	0.95	0
3	BMA	D	804	3	11,11,12	0.59	0	14,15,17	0.86	0
3	MAN	D	805	3	11,11,12	0.43	0	14,15,17	2.95	5 (35%)
3	MAN	D	806	3	11,11,12	0.67	0	14,15,17	2.19	5 (35%)
8	NAG	D	808	1,8	14,14,15	0.44	0	15,19,21	1.50	3 (20%)
8	FUL	D	809	8	10,10,11	0.67	0	14,14,16	1.57	3 (21%)

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	SIA	A	801	2	-	0/14/34/38	0/1/1/1
2	GAL	A	802	2	-	0/2/22/22	0/1/1/1
3	NAG	A	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	804	3	-	0/6/23/26	0/1/1/1
3	BMA	A	805	3	-	0/2/19/22	0/1/1/1
3	MAN	A	806	3	-	0/2/19/22	0/1/1/1
3	MAN	A	807	3	-	0/2/19/22	0/1/1/1
2	SIA	B	801	2	-	0/14/34/38	0/1/1/1
2	GAL	B	802	2	-	0/2/22/22	0/1/1/1
3	NAG	B	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	804	3	-	0/6/23/26	0/1/1/1
3	BMA	B	805	3	-	0/2/19/22	0/1/1/1
3	MAN	B	806	3	-	0/2/19/22	0/1/1/1
3	MAN	B	807	3	-	0/2/19/22	0/1/1/1
3	NAG	C	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	803	3	-	0/6/23/26	0/1/1/1
3	BMA	C	804	3	-	0/2/19/22	0/1/1/1
3	MAN	C	805	3	-	0/2/19/22	0/1/1/1
3	MAN	C	806	3	-	0/2/19/22	0/1/1/1
7	NAG	C	807	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	808	7	-	0/6/23/26	0/1/1/1
7	FUC	C	809	7	-	0/0/17/20	0/1/1/1
3	NAG	D	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	3	-	0/6/23/26	0/1/1/1
3	BMA	D	804	3	-	0/2/19/22	0/1/1/1
3	MAN	D	805	3	-	0/2/19/22	0/1/1/1
3	MAN	D	806	3	-	0/2/19/22	0/1/1/1
8	NAG	D	808	1,8	-	0/6/23/26	0/1/1/1
8	FUL	D	809	8	-	0/0/17/20	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SIA	C7-C6	2.19	1.55	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	809	FUL	C1-O5-C5	-3.52	106.94	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	805	MAN	C3-C4-C5	-3.32	104.41	110.20
3	D	805	MAN	C2-C3-C4	-3.24	105.54	111.04
3	C	805	MAN	C3-C4-C5	-3.07	104.84	110.20
2	B	802	GAL	C1-C2-C3	-3.07	105.86	110.43
3	A	806	MAN	C3-C4-C5	-3.04	104.90	110.20
3	B	804	NAG	C2-N2-C7	-3.00	119.19	123.04
8	D	809	FUL	C1-C2-C3	-2.92	106.09	109.54
3	A	804	NAG	O7-C7-C8	-2.74	117.04	122.06
3	A	805	BMA	O6-C6-C5	-2.45	103.22	111.33
3	B	804	NAG	C3-C4-C5	-2.44	105.95	110.20
3	C	803	NAG	C3-C4-C5	-2.40	106.01	110.20
2	B	801	SIA	C7-C6-C5	-2.30	110.85	114.32
3	B	804	NAG	O4-C4-C3	-2.28	105.20	110.34
8	D	808	NAG	O3-C3-C2	-2.28	104.60	109.11
3	A	804	NAG	O4-C4-C3	-2.22	105.34	110.34
7	C	807	NAG	C3-C2-N2	-2.14	105.44	110.56
3	C	803	NAG	C2-N2-C7	2.00	125.61	123.04
2	A	801	SIA	O7-C7-C8	2.03	113.86	108.75
2	A	802	GAL	C3-C4-C5	2.07	113.80	110.20
3	C	805	MAN	O4-C4-C5	2.14	114.90	109.24
3	B	806	MAN	O5-C1-C2	2.15	114.34	110.86
2	B	801	SIA	O6-C2-C3	2.20	114.09	109.86
3	A	806	MAN	C1-O5-C5	2.29	115.15	112.25
3	D	805	MAN	O3-C3-C4	2.33	115.59	110.34
3	A	804	NAG	C4-C3-C2	2.41	114.98	111.23
3	A	803	NAG	O3-C3-C2	2.49	114.05	109.11
3	D	806	MAN	O5-C5-C6	2.65	113.08	107.35
3	C	805	MAN	C1-O5-C5	2.69	115.66	112.25
8	D	809	FUL	O5-C5-C6	2.74	110.66	106.13
2	B	802	GAL	C1-O5-C5	2.77	118.59	113.47
8	D	808	NAG	C4-C3-C2	2.78	115.55	111.23
3	C	806	MAN	C2-C3-C4	2.93	116.02	111.04
3	C	803	NAG	O5-C5-C6	3.02	113.88	107.35
8	D	808	NAG	C1-O5-C5	3.15	116.24	112.25
3	D	805	MAN	O5-C1-C2	3.19	116.03	110.86
3	D	806	MAN	C1-O5-C5	3.19	116.30	112.25
2	B	802	GAL	C3-C4-C5	3.25	115.87	110.20
2	A	801	SIA	O6-C2-C3	3.27	116.15	109.86
3	B	807	MAN	O5-C1-C2	3.27	116.17	110.86
7	C	809	FUC	O5-C5-C6	3.35	111.67	106.13
3	A	803	NAG	C1-O5-C5	3.51	116.70	112.25
7	C	808	NAG	C4-C3-C2	3.59	116.81	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	807	MAN	C1-C2-C3	3.68	113.89	109.54
3	D	806	MAN	C3-C4-C5	3.80	116.81	110.20
3	A	807	MAN	O5-C1-C2	3.88	117.16	110.86
3	D	806	MAN	C2-C3-C4	3.94	117.73	111.04
3	C	806	MAN	O5-C1-C2	4.03	117.39	110.86
7	C	807	NAG	C4-C3-C2	4.15	117.67	111.23
3	D	806	MAN	C1-C2-C3	4.15	114.46	109.54
2	B	802	GAL	O5-C5-C4	4.53	118.18	109.68
3	A	807	MAN	C1-O5-C5	5.05	118.66	112.25
3	A	807	MAN	C1-C2-C3	5.51	116.06	109.54
3	B	806	MAN	C1-O5-C5	5.98	119.83	112.25
3	C	806	MAN	C1-O5-C5	6.31	120.25	112.25
3	C	806	MAN	C1-C2-C3	7.31	118.18	109.54
3	B	807	MAN	C1-O5-C5	7.44	121.70	112.25
3	D	805	MAN	C1-O5-C5	8.30	122.78	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	NAG	1	0
3	C	804	BMA	1	0
7	C	809	FUC	1	0
3	D	802	NAG	1	0
8	D	808	NAG	1	0

## 5.6 Ligand geometry

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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
4	NAG	A	808	1	14,14,15	0.52	0	15,19,21	1.47	3 (20%)
4	NAG	A	809	1	14,14,15	0.51	0	15,19,21	1.46	2 (13%)
4	NAG	A	810	1	14,14,15	0.45	0	15,19,21	1.23	1 (6%)
4	NAG	B	808	1	14,14,15	0.46	0	15,19,21	1.50	2 (13%)
4	NAG	B	809	1	14,14,15	0.45	0	15,19,21	1.52	2 (13%)
4	NAG	B	810	1	14,14,15	0.48	0	15,19,21	1.78	1 (6%)
6	SIA	C	801	-	17,21,21	1.39	3 (17%)	19,31,31	1.46	3 (15%)
4	NAG	C	810	1	14,14,15	0.70	1 (7%)	15,19,21	1.57	3 (20%)
4	NAG	C	811	1	14,14,15	0.66	0	15,19,21	1.46	2 (13%)
6	SIA	D	801	-	17,21,21	1.07	3 (17%)	19,31,31	1.88	5 (26%)
4	NAG	D	807	1	14,14,15	0.48	0	15,19,21	1.88	1 (6%)
4	NAG	D	810	1	14,14,15	0.50	0	15,19,21	1.49	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	808	1	-	0/6/23/26	0/1/1/1
4	NAG	A	809	1	-	0/6/23/26	0/1/1/1
4	NAG	A	810	1	-	0/6/23/26	0/1/1/1
4	NAG	B	808	1	-	0/6/23/26	0/1/1/1
4	NAG	B	809	1	-	0/6/23/26	0/1/1/1
4	NAG	B	810	1	-	0/6/23/26	0/1/1/1
6	SIA	C	801	-	-	0/14/38/38	0/1/1/1
4	NAG	C	810	1	-	0/6/23/26	0/1/1/1
4	NAG	C	811	1	-	0/6/23/26	0/1/1/1
6	SIA	D	801	-	-	0/14/38/38	0/1/1/1
4	NAG	D	807	1	-	0/6/23/26	0/1/1/1
4	NAG	D	810	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	801	SIA	O6-C2	2.06	1.44	1.42
4	C	810	NAG	C1-C2	2.13	1.55	1.52
6	C	801	SIA	C3-C2	2.21	1.54	1.51
6	D	801	SIA	C3-C2	2.30	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	801	SIA	O6-C2	2.45	1.45	1.42
6	D	801	SIA	O2-C2	2.58	1.42	1.40
6	C	801	SIA	O2-C2	4.73	1.45	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	801	SIA	O2-C2-C3	-5.62	102.39	109.41
4	D	810	NAG	C4-C3-C2	-3.47	105.84	111.23
6	C	801	SIA	O2-C2-C3	-3.43	105.13	109.41
6	D	801	SIA	C7-C6-C5	-3.15	109.55	114.32
6	C	801	SIA	C7-C6-C5	-2.76	110.14	114.32
4	C	810	NAG	C4-C3-C2	-2.76	106.94	111.23
4	B	809	NAG	O3-C3-C2	-2.69	103.78	109.11
4	C	810	NAG	C3-C4-C5	-2.26	106.25	110.20
4	A	809	NAG	O3-C3-C2	-2.22	104.72	109.11
4	A	808	NAG	C1-O5-C5	2.03	114.82	112.25
6	D	801	SIA	C6-C5-N5	2.11	114.74	111.07
4	D	810	NAG	C1-O5-C5	2.11	114.93	112.25
4	A	808	NAG	C4-C3-C2	2.13	114.53	111.23
4	D	810	NAG	O3-C3-C2	2.15	113.37	109.11
6	D	801	SIA	C2-C3-C4	2.35	115.75	110.69
4	B	808	NAG	C3-C4-C5	2.48	114.52	110.20
4	C	811	NAG	C1-O5-C5	2.54	115.47	112.25
6	D	801	SIA	O2-C2-O6	2.62	114.49	110.22
6	C	801	SIA	C2-C3-C4	2.78	116.68	110.69
4	C	811	NAG	C4-C3-C2	3.05	115.97	111.23
4	C	810	NAG	C1-O5-C5	3.44	116.61	112.25
4	A	809	NAG	C1-O5-C5	3.67	116.90	112.25
4	A	810	NAG	C1-O5-C5	3.93	117.23	112.25
4	B	809	NAG	C1-O5-C5	4.30	117.70	112.25
4	A	808	NAG	C3-C4-C5	4.37	117.81	110.20
4	B	808	NAG	C1-O5-C5	4.43	117.86	112.25
4	B	810	NAG	C1-O5-C5	6.52	120.52	112.25
4	D	807	NAG	C1-O5-C5	6.64	120.67	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	809	NAG	1	0
4	A	810	NAG	1	0
4	B	809	NAG	2	0
4	B	810	NAG	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/393 (98%)	0.24	10 (2%) 59 62	15, 26, 40, 56	0
1	B	388/393 (98%)	0.35	14 (3%) 46 50	15, 27, 40, 57	0
1	C	388/393 (98%)	0.26	14 (3%) 46 50	15, 26, 40, 59	0
1	D	388/393 (98%)	0.18	11 (2%) 56 60	16, 26, 40, 57	0
All	All	1552/1572 (98%)	0.26	49 (3%) 51 54	15, 26, 40, 59	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	ILE	8.5
1	A	469	ILE	7.0
1	D	468	PRO	5.9
1	D	469	ILE	5.7
1	C	468	PRO	4.9
1	B	469	ILE	4.6
1	A	468	PRO	4.3
1	A	431	LYS	3.5
1	A	330	ASP	3.3
1	D	82	ALA	3.0
1	C	463	ASP	2.9
1	B	82	ALA	2.9
1	D	308	LYS	2.8
1	D	86	ASN	2.7
1	D	465	ASN	2.7
1	C	114	ILE	2.6
1	B	468	PRO	2.6
1	B	86	ASN	2.6
1	D	83	GLU	2.6
1	B	165	VAL	2.6
1	C	369	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	369	THR	2.5
1	B	83	GLU	2.5
1	C	390	LEU	2.5
1	D	467	MET	2.5
1	B	337	CYS	2.4
1	B	369	THR	2.4
1	A	400	ARG	2.4
1	B	159	LEU	2.3
1	B	168	HIS	2.3
1	D	463	ASP	2.3
1	B	247	SER	2.3
1	C	318	CYS	2.3
1	C	344	GLU	2.2
1	C	330	ASP	2.2
1	A	169	LEU	2.2
1	A	337	CYS	2.2
1	B	167	PHE	2.2
1	C	337	CYS	2.2
1	B	270	GLY	2.2
1	A	150	ARG	2.2
1	B	331	SER	2.1
1	D	332	SER	2.1
1	C	86	ASN	2.1
1	C	147	ASN	2.1
1	C	400	ARG	2.1
1	A	344	GLU	2.0
1	C	465	ASN	2.0
1	D	330	ASP	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SIA	B	801	20/21	0.86	0.17	0.73	37,42,44,44	0
3	NAG	B	803	14/15	0.89	0.19	0.60	20,32,36,36	0
3	NAG	D	802	14/15	0.90	0.17	0.42	23,31,33,34	0
2	SIA	A	801	20/21	0.89	0.18	0.31	30,40,44,45	0
3	NAG	A	803	14/15	0.89	0.16	-0.00	29,33,37,38	0
3	NAG	C	802	14/15	0.90	0.15	-0.46	28,33,35,35	0
7	FUC	C	809	10/11	0.76	0.29	-	66,66,67,67	0
3	MAN	D	805	11/12	0.73	0.23	-	48,49,50,51	0
3	BMA	C	804	11/12	0.88	0.19	-	41,43,46,49	0
8	NAG	D	808	14/15	0.82	0.22	-	49,53,56,57	0
3	NAG	D	803	14/15	0.90	0.18	-	30,33,35,39	0
7	NAG	C	808	14/15	0.69	0.30	-	66,68,71,72	0
3	MAN	A	807	11/12	0.72	0.28	-	47,48,50,50	0
7	NAG	C	807	14/15	0.75	0.19	-	56,60,65,65	0
3	NAG	C	803	14/15	0.92	0.14	-	34,35,36,38	0
3	MAN	B	806	11/12	0.80	0.20	-	40,43,44,46	0
3	BMA	A	805	11/12	0.78	0.21	-	41,43,45,47	0
8	FUL	D	809	10/11	0.65	0.37	-	59,60,61,61	0
2	GAL	A	802	12/12	0.63	0.28	-	54,63,64,64	0
3	MAN	D	806	11/12	0.72	0.25	-	52,54,56,56	0
3	BMA	B	805	11/12	0.78	0.21	-	40,42,45,49	0
3	MAN	C	806	11/12	0.74	0.24	-	52,53,54,55	0
3	MAN	A	806	11/12	0.80	0.26	-	39,43,45,46	0
3	BMA	D	804	11/12	0.92	0.15	-	42,45,47,50	0
3	NAG	A	804	14/15	0.91	0.15	-	36,37,39,40	0
2	GAL	B	802	12/12	0.50	0.39	-	55,66,67,67	0
3	MAN	C	805	11/12	0.86	0.20	-	46,46,48,51	0
3	MAN	B	807	11/12	0.73	0.28	-	49,50,50,52	0
3	NAG	B	804	14/15	0.87	0.18	-	33,35,38,39	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	810	14/15	0.74	0.31	2.11	48,50,54,55	0
6	SIA	D	801	21/21	0.87	0.20	1.25	33,38,39,40	0
6	SIA	C	801	21/21	0.86	0.19	0.99	29,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	811	14/15	0.77	0.23	-0.16	45,48,52,53	0
5	CA	B	811	1/1	0.94	0.07	-2.01	32,32,32,32	0
5	CA	C	812	1/1	0.95	0.06	-2.32	38,38,38,38	0
5	CA	A	812	1/1	0.98	0.07	-2.33	31,31,31,31	0
5	CA	D	811	1/1	0.96	0.06	-3.97	40,40,40,40	0
4	NAG	A	810	14/15	0.83	0.31	-	47,48,50,50	0
4	NAG	D	807	14/15	0.72	0.33	-	52,55,58,58	0
4	NAG	A	809	14/15	0.79	0.18	-	56,60,67,67	0
4	NAG	B	809	14/15	0.69	0.24	-	52,55,61,61	0
4	NAG	A	808	14/15	0.82	0.24	-	55,57,58,58	0
4	NAG	D	810	14/15	0.79	0.29	-	46,47,48,49	0
4	NAG	C	810	14/15	0.71	0.36	-	45,49,50,52	0
4	NAG	B	808	14/15	0.65	0.27	-	56,59,60,60	0
5	CA	A	811	1/1	0.53	0.20	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.