



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:06 PM GMT

PDB ID : 3D26  
Title : Norwalk P domain A-trisaccharide complex  
Authors : Hegde, R.; Bu, W.  
Deposited on : 2008-05-07  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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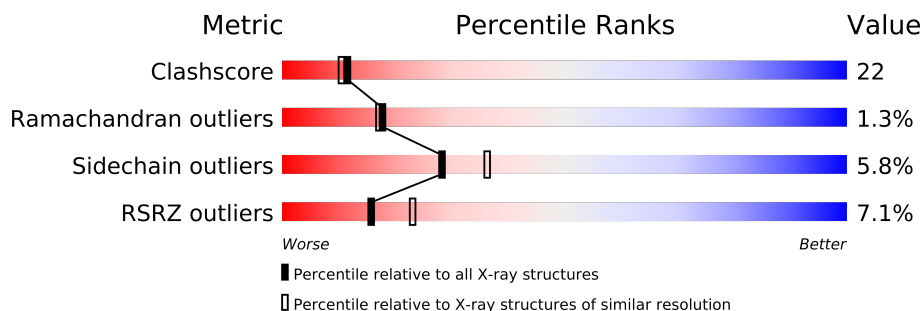
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4540 atoms, of which 0 are hydrogen and 0 are deuterium.

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 58 kd capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2138	1372	355	403	8			
1	B	284	Total	C	N	O	S	0	0	0
			2142	1375	355	404	8			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			36	20	1	15		
2	B	3	Total	C	N	O	0	0
			36	20	1	15		

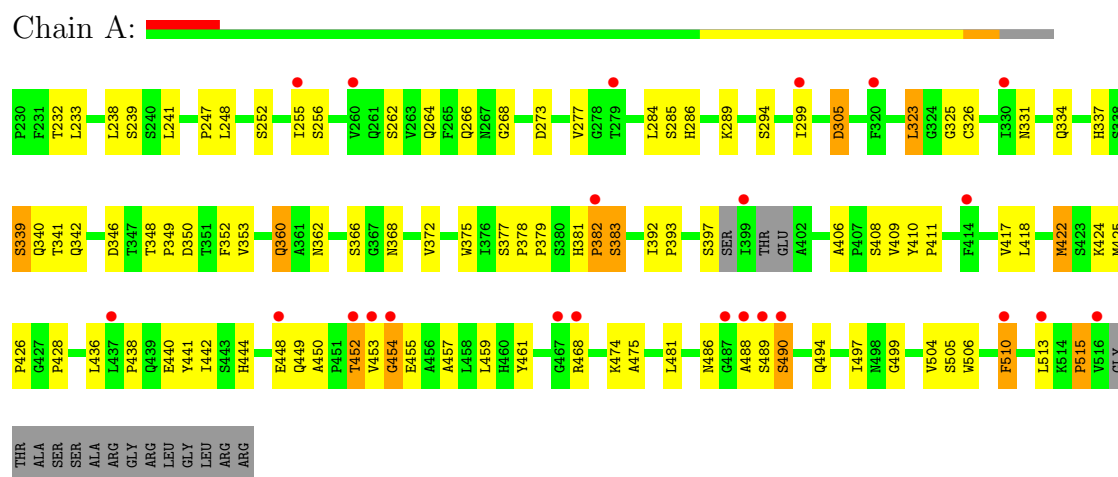
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	140	Total	O	0	0
			140	140		

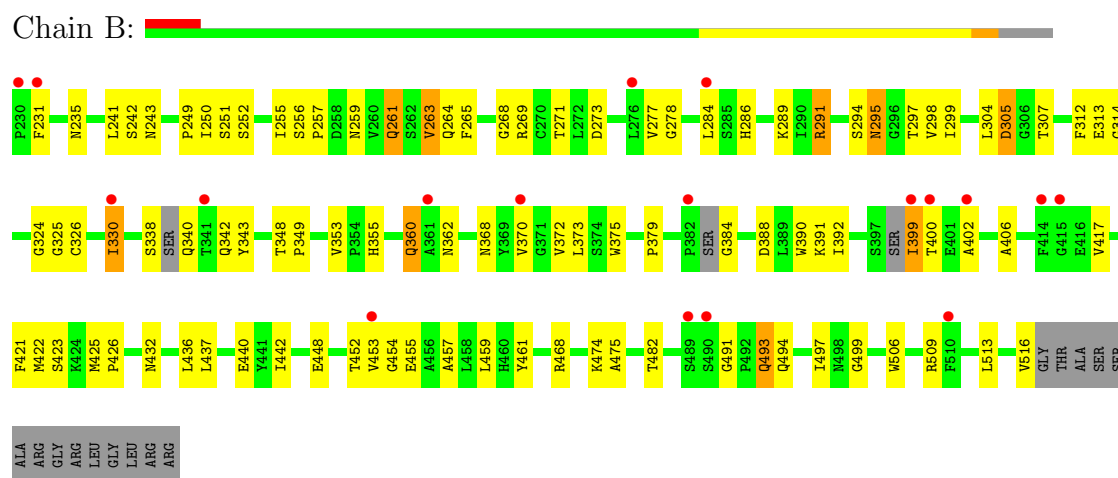
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 58 kd capsid protein



- Molecule 1: 58 kd capsid protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.01Å 83.01Å 162.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 65.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 88.6 (65.77-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.10 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.220 , 0.260 0.257 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 12.0	EDS
Estimated twinning fraction	0.084 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 26421 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4540	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NGA, 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	0.38	0/2208	0.69	1/3027 (0.0%)
1	B	0.36	0/2211	0.67	0/3030
All	All	0.37	0/4419	0.68	1/6057 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	2	0
2	B	1	0
All	All	3	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	PRO	N-CA-C	-5.82	96.96	112.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	531	NGA	C1
2	A	532	GAL	C3
2	B	531	NGA	C1

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2138	0	2058	98	0
1	B	2142	0	2060	98	0
2	A	36	0	33	0	0
2	B	36	0	33	2	0
3	A	48	0	0	9	0
3	B	140	0	0	14	0
All	All	4540	0	4184	188	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (188) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:241:LEU:HD22	1:A:440:GLU:HG3	1.26	1.09
1:A:266:GLN:HG2	1:A:392:ILE:HD11	1.35	1.06
1:B:261:GLN:HA	1:B:261:GLN:HE21	1.30	0.95
1:B:452:THR:HG22	3:B:714:HOH:O	1.72	0.90
1:B:241:LEU:HD22	1:B:440:GLU:HG3	1.54	0.88
1:B:295:ASN:ND2	1:B:297:THR:H	1.76	0.84
1:A:422:MET:HB2	3:A:540:HOH:O	1.79	0.80
1:A:474:LYS:HG3	1:A:513:LEU:HD21	1.66	0.77
1:A:449:GLN:HE22	1:B:235:ASN:ND2	1.83	0.76
1:A:241:LEU:HD22	1:A:440:GLU:CG	2.09	0.76
1:A:453:VAL:HG12	1:A:454:GLY:H	1.53	0.74
1:A:340:GLN:HG2	1:B:342:GLN:HE21	1.54	0.73
1:B:295:ASN:HD21	1:B:298:VAL:H	1.35	0.73
1:B:259:ASN:ND2	3:B:613:HOH:O	2.21	0.73
1:B:273:ASP:HB2	3:B:583:HOH:O	1.89	0.72
1:A:341:THR:HG23	3:A:556:HOH:O	1.89	0.72
1:A:266:GLN:CG	1:A:392:ILE:HD11	2.17	0.72
1:A:381:HIS:O	1:A:383:SER:N	2.22	0.71
1:B:360:GLN:NE2	1:B:360:GLN:H	1.88	0.71
2:B:531:NGA:H5	2:B:533:FUC:O2	1.91	0.70
1:B:268:GLY:HA2	1:B:442:ILE:HD11	1.73	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:GLN:H	1:A:360:GLN:HE21	1.41	0.67
1:B:295:ASN:HD22	1:B:297:THR:H	1.41	0.67
1:A:252:SER:HA	1:A:497:ILE:HG21	1.75	0.67
1:B:330:ILE:HG22	1:B:373:LEU:HA	1.78	0.66
1:A:490:SER:HB2	1:A:494:GLN:OE1	1.95	0.65
1:B:305:ASP:HB3	1:B:307:THR:HG23	1.77	0.65
1:B:491:GLY:N	1:B:493:GLN:HE21	1.94	0.64
1:A:247:PRO:HB3	1:A:284:LEU:HD11	1.78	0.64
1:A:264:GLN:O	1:A:392:ILE:HD12	1.97	0.63
1:A:425:MET:CE	1:A:426:PRO:HD2	2.28	0.63
1:B:459:LEU:HD11	1:B:475:ALA:HB2	1.81	0.62
1:B:360:GLN:HE21	1:B:360:GLN:H	1.47	0.62
1:A:360:GLN:NE2	1:A:360:GLN:H	1.97	0.62
1:B:425:MET:CE	1:B:426:PRO:HD2	2.29	0.62
1:B:295:ASN:HD22	1:B:295:ASN:C	2.03	0.62
1:B:291:ARG:HE	1:B:368:ASN:HD21	1.47	0.62
1:B:295:ASN:ND2	1:B:298:VAL:H	1.97	0.61
1:B:436:LEU:O	1:B:437:LEU:HD23	2.00	0.61
1:A:381:HIS:C	1:A:383:SER:N	2.53	0.61
3:A:535:HOH:O	1:B:286:HIS:HE1	1.82	0.61
1:B:474:LYS:HG3	1:B:513:LEU:HD21	1.82	0.61
1:A:331:ASN:HD21	1:A:340:GLN:HB2	1.65	0.60
1:B:264:GLN:NE2	3:B:603:HOH:O	2.34	0.60
1:A:241:LEU:CD2	1:A:440:GLU:HG3	2.18	0.59
1:A:342:GLN:HE21	1:B:340:GLN:HG2	1.68	0.59
1:B:425:MET:HE3	1:B:426:PRO:HD2	1.85	0.59
1:A:232:THR:HG22	1:A:444:HIS:CE1	2.38	0.58
1:B:392:ILE:O	1:B:392:ILE:HD12	2.04	0.58
1:A:339:SER:HA	1:B:375:TRP:CZ2	2.38	0.58
2:B:531:NGA:H62	3:B:692:HOH:O	2.03	0.58
1:A:425:MET:HE3	1:A:426:PRO:HD2	1.86	0.58
1:B:452:THR:HG21	3:B:583:HOH:O	2.04	0.57
1:A:239:SER:HB3	1:A:497:ILE:HD13	1.86	0.57
1:B:326:CYS:HA	1:B:379:PRO:HG3	1.86	0.57
1:A:255:ILE:HG22	1:A:256:SER:N	2.19	0.57
1:A:457:ALA:HB2	1:A:506:TRP:CZ3	2.39	0.57
1:A:294:SER:O	1:A:366:SER:HA	2.04	0.57
1:B:261:GLN:HA	1:B:261:GLN:NE2	2.09	0.56
1:B:330:ILE:HD11	1:B:343:TYR:CD2	2.41	0.56
1:A:486:ASN:HD21	1:A:515:PRO:HB2	1.71	0.56
1:A:383:SER:HB2	3:A:538:HOH:O	2.06	0.56
1:B:252:SER:HA	1:B:497:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:VAL:HG12	1:B:454:GLY:N	2.20	0.55
1:A:285:SER:HB3	1:B:242:SER:HB2	1.88	0.55
1:B:241:LEU:CD2	1:B:440:GLU:HG3	2.32	0.55
1:B:330:ILE:HG22	1:B:373:LEU:CA	2.36	0.54
1:A:284:LEU:HD13	1:A:284:LEU:O	2.09	0.53
1:B:291:ARG:HH11	1:B:291:ARG:HG3	1.74	0.53
1:B:353:VAL:HG23	1:B:353:VAL:O	2.09	0.53
1:A:233:LEU:HD22	1:A:441:TYR:CE2	2.44	0.53
1:A:252:SER:HA	1:A:497:ILE:CG2	2.39	0.53
1:B:256:SER:HA	1:B:390:TRP:CH2	2.44	0.53
1:A:323:LEU:N	1:A:323:LEU:HD23	2.23	0.53
1:A:489:SER:O	1:A:490:SER:HB2	2.09	0.52
1:B:251:SER:O	1:B:497:ILE:HG21	2.08	0.52
1:A:353:VAL:HG11	1:A:397:SER:HB3	1.91	0.52
1:A:348:THR:N	1:A:349:PRO:HD2	2.24	0.52
1:B:243:ASN:HB2	1:B:423:SER:OG	2.10	0.52
1:B:375:TRP:HA	1:B:425:MET:CE	2.39	0.52
1:A:289:LYS:HG2	1:A:372:VAL:HG13	1.92	0.52
1:A:268:GLY:HA2	1:A:442:ILE:HD11	1.91	0.52
1:A:449:GLN:N	3:A:537:HOH:O	2.42	0.52
1:A:449:GLN:HE22	1:B:235:ASN:HD22	1.53	0.51
1:A:255:ILE:HG23	1:A:417:VAL:CG1	2.40	0.51
1:A:352:PHE:O	3:A:543:HOH:O	2.19	0.51
1:A:449:GLN:NE2	1:B:235:ASN:HD22	2.08	0.51
1:B:417:VAL:O	1:B:482:THR:HA	2.11	0.51
1:A:504:VAL:O	1:A:505:SER:HB3	2.10	0.51
1:B:468:ARG:HB3	1:B:468:ARG:NH1	2.26	0.51
1:A:449:GLN:NE2	1:B:235:ASN:ND2	2.56	0.51
1:B:491:GLY:CA	1:B:493:GLN:HE21	2.24	0.50
1:A:379:PRO:HB2	1:A:382:PRO:HD2	1.93	0.50
1:A:268:GLY:HA2	1:A:442:ILE:CD1	2.42	0.50
1:A:490:SER:HB2	1:A:494:GLN:CD	2.31	0.50
1:B:289:LYS:HG2	1:B:372:VAL:HG22	1.92	0.50
1:A:286:HIS:HE1	3:B:612:HOH:O	1.93	0.50
1:B:330:ILE:HG13	1:B:343:TYR:HB3	1.93	0.50
1:A:409:VAL:HG21	1:A:436:LEU:HD11	1.94	0.49
1:B:277:VAL:HG12	1:B:406:ALA:CB	2.41	0.49
1:A:248:LEU:HD13	1:A:424:LYS:O	2.13	0.49
1:B:348:THR:N	1:B:349:PRO:HD2	2.27	0.49
1:B:455:GLU:HG2	1:B:509:ARG:NH2	2.26	0.49
1:A:348:THR:N	1:A:349:PRO:CD	2.75	0.48
1:B:330:ILE:HG22	1:B:373:LEU:N	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:CYS:N	1:B:379:PRO:HG3	2.29	0.48
1:B:295:ASN:ND2	1:B:295:ASN:C	2.65	0.48
1:A:381:HIS:C	1:A:383:SER:H	2.11	0.48
1:B:468:ARG:HH11	1:B:468:ARG:HB3	1.79	0.48
1:A:392:ILE:HG12	1:A:393:PRO:HD2	1.95	0.47
1:B:255:ILE:HG23	3:B:581:HOH:O	2.14	0.47
1:A:453:VAL:HG12	1:A:454:GLY:N	2.25	0.47
1:A:379:PRO:CB	1:A:382:PRO:HD2	2.44	0.47
1:A:247:PRO:CB	1:A:284:LEU:HD11	2.43	0.47
1:B:314:GLY:O	1:B:355:HIS:HD2	1.96	0.47
1:A:334:GLN:HB2	1:A:337:HIS:HB2	1.96	0.47
1:A:510:PHE:CD1	1:A:510:PHE:N	2.82	0.47
1:A:277:VAL:HG12	1:A:406:ALA:HB1	1.96	0.47
1:A:461:TYR:CZ	1:A:499:GLY:HA3	2.49	0.47
1:A:342:GLN:NE2	1:A:375:TRP:HE1	2.13	0.46
1:B:388:ASP:OD2	1:B:391:LYS:HE3	2.15	0.46
1:A:438:PRO:O	1:A:441:TYR:HB2	2.15	0.46
1:B:399:ILE:N	1:B:399:ILE:HD12	2.30	0.46
1:A:411:PRO:HG3	1:A:418:LEU:CD1	2.46	0.46
1:A:468:ARG:HG2	1:A:468:ARG:HH11	1.81	0.46
1:A:450:ALA:O	1:A:452:THR:N	2.48	0.46
1:B:268:GLY:HA2	1:B:442:ILE:CD1	2.43	0.45
1:B:417:VAL:HG12	3:B:581:HOH:O	2.16	0.45
1:A:233:LEU:HD22	1:A:441:TYR:CD2	2.51	0.45
1:A:457:ALA:HB3	1:A:475:ALA:HB3	1.98	0.45
1:B:294:SER:HB2	1:B:299:ILE:HG12	1.97	0.45
1:A:305:ASP:HB2	3:A:564:HOH:O	2.16	0.45
1:A:428:PRO:HB3	1:B:338:SER:OG	2.16	0.45
1:A:453:VAL:O	1:A:454:GLY:O	2.35	0.45
1:A:486:ASN:ND2	1:A:515:PRO:HB2	2.32	0.45
1:B:509:ARG:NH1	3:B:620:HOH:O	2.49	0.45
1:B:375:TRP:HA	1:B:425:MET:HE1	1.98	0.45
1:B:255:ILE:HG22	1:B:256:SER:N	2.31	0.45
1:B:324:GLY:HA2	3:B:628:HOH:O	2.18	0.45
1:A:360:GLN:O	1:A:360:GLN:HG2	2.16	0.44
1:A:289:LYS:HE3	1:A:372:VAL:HG22	1.98	0.44
1:A:232:THR:CG2	1:A:233:LEU:N	2.80	0.44
1:B:455:GLU:HB3	1:B:509:ARG:HB2	2.00	0.44
1:B:493:GLN:H	1:B:493:GLN:HG3	1.31	0.44
1:B:491:GLY:O	1:B:494:GLN:HG2	2.17	0.44
1:B:325:GLY:O	1:B:326:CYS:HB3	2.17	0.44
1:B:263:VAL:HG22	1:B:265:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:262:SER:HB3	1:A:410:TYR:CD1	2.51	0.44
1:B:277:VAL:HG12	1:B:406:ALA:HB2	1.99	0.44
1:A:264:GLN:HB2	1:A:408:SER:HB3	2.00	0.44
1:B:326:CYS:CA	1:B:379:PRO:HG3	2.47	0.44
1:A:334:GLN:HG2	1:A:368:ASN:O	2.17	0.44
1:B:457:ALA:HB2	1:B:506:TRP:CZ3	2.52	0.44
1:B:291:ARG:NH1	1:B:291:ARG:HG3	2.32	0.44
1:B:269:ARG:HA	3:B:587:HOH:O	2.17	0.44
1:A:490:SER:CB	1:A:494:GLN:OE1	2.64	0.44
1:B:291:ARG:NE	1:B:368:ASN:HD21	2.13	0.43
1:B:425:MET:HE2	1:B:426:PRO:HD2	1.99	0.43
1:B:330:ILE:HG12	1:B:330:ILE:H	1.59	0.43
1:A:294:SER:HB2	1:A:299:ILE:HG12	1.99	0.43
1:B:271:THR:OG1	1:B:273:ASP:HB3	2.19	0.43
1:B:330:ILE:CG2	1:B:373:LEU:HA	2.48	0.43
1:A:488:ALA:C	1:A:490:SER:N	2.72	0.43
1:A:425:MET:HE2	1:A:426:PRO:HD2	2.00	0.43
1:A:286:HIS:HD2	3:A:574:HOH:O	2.02	0.43
1:A:331:ASN:ND2	1:A:340:GLN:HB2	2.30	0.43
1:B:375:TRP:HA	1:B:425:MET:HE2	2.01	0.42
1:A:409:VAL:HG21	1:A:436:LEU:CD1	2.50	0.42
1:B:250:ILE:HD12	1:B:421:PHE:HB3	2.02	0.42
1:B:257:PRO:HD3	1:B:390:TRP:CE2	2.55	0.42
1:A:346:ASP:O	1:A:349:PRO:HD2	2.20	0.42
1:B:271:THR:HG1	1:B:273:ASP:HB3	1.84	0.42
1:B:491:GLY:N	1:B:493:GLN:NE2	2.66	0.42
1:A:255:ILE:HG22	1:A:256:SER:H	1.83	0.41
1:A:286:HIS:CE1	3:B:612:HOH:O	2.72	0.41
1:A:448:GLU:C	3:A:537:HOH:O	2.59	0.41
1:B:312:PHE:CE1	1:B:313:GLU:HG3	2.56	0.41
1:A:377:SER:HB2	1:A:378:PRO:CD	2.50	0.41
1:B:384:GLY:N	3:B:694:HOH:O	2.54	0.41
1:B:461:TYR:CZ	1:B:499:GLY:HA3	2.56	0.41
1:A:474:LYS:O	1:A:481:LEU:HA	2.21	0.41
1:A:286:HIS:CE1	1:B:249:PRO:HB3	2.55	0.41
1:B:257:PRO:HD3	1:B:390:TRP:CZ2	2.56	0.40
1:A:325:GLY:O	1:A:326:CYS:HB3	2.21	0.40
1:B:291:ARG:HG2	1:B:370:VAL:HG22	2.03	0.40
1:A:459:LEU:HD11	1:A:475:ALA:HB2	2.03	0.40
1:A:348:THR:H	1:A:349:PRO:CD	2.34	0.40
1:B:277:VAL:HG12	1:B:278:GLY:N	2.36	0.40

There are no symmetry-related clashes.

## 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	279/301 (93%)	253 (91%)	21 (8%)	5 (2%)	13	10
1	B	276/301 (92%)	261 (95%)	13 (5%)	2 (1%)	30	34
All	All	555/602 (92%)	514 (93%)	34 (6%)	7 (1%)	18	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	GLY
1	A	490	SER
1	B	231	PHE
1	B	402	ALA
1	A	339	SER
1	A	383	SER
1	A	515	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	240/253 (95%)	229 (95%)	11 (5%)	37	48
1	B	240/253 (95%)	223 (93%)	17 (7%)	21	26
All	All	480/506 (95%)	452 (94%)	28 (6%)	28	36

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LEU
1	A	273	ASP

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Mol	Chain	Res	Type
1	A	305	ASP
1	A	323	LEU
1	A	350	ASP
1	A	360	GLN
1	A	362	ASN
1	A	422	MET
1	A	452	THR
1	A	455	GLU
1	A	510	PHE
1	B	261	GLN
1	B	263	VAL
1	B	284	LEU
1	B	291	ARG
1	B	295	ASN
1	B	304	LEU
1	B	305	ASP
1	B	330	ILE
1	B	360	GLN
1	B	362	ASN
1	B	399	ILE
1	B	400	THR
1	B	422	MET
1	B	432	ASN
1	B	448	GLU
1	B	493	GLN
1	B	516	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	286	HIS
1	A	331	ASN
1	A	342	GLN
1	A	360	GLN
1	A	362	ASN
1	A	381	HIS
1	A	394	ASN
1	A	486	ASN
1	A	498	ASN
1	B	235	ASN
1	B	261	GLN

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Mol	Chain	Res	Type
1	B	286	HIS
1	B	295	ASN
1	B	342	GLN
1	B	355	HIS
1	B	360	GLN
1	B	362	ASN
1	B	368	ASN
1	B	449	GLN
1	B	469	ASN
1	B	493	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	NGA	A	531	2	12,14,15	0.60	0	15,19,21	1.04	1 (6%)
2	GAL	A	532	2	11,11,12	0.69	0	10,15,17	1.38	2 (20%)
2	FUC	A	533	2	11,11,11	0.52	0	16,16,16	0.81	0
2	NGA	B	531	2	12,14,15	0.56	0	15,19,21	0.99	1 (6%)
2	GAL	B	532	2	11,11,12	0.75	0	10,15,17	1.64	2 (20%)
2	FUC	B	533	2	11,11,11	0.54	0	16,16,16	0.99	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	NGA	A	531	2	1/1/5/7	0/6/23/26	0/1/1/1
2	GAL	A	532	2	1/1/4/5	0/2/18/22	0/1/1/1
2	FUC	A	533	2	-	0/0/20/20	0/1/1/1
2	NGA	B	531	2	1/1/5/7	0/6/23/26	0/1/1/1
2	GAL	B	532	2	-	0/2/18/22	0/1/1/1
2	FUC	B	533	2	-	0/0/20/20	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	GAL	O1-C1-O5	-4.09	107.13	111.54
2	A	532	GAL	C1-O5-C5	-3.22	109.12	113.47
2	A	531	NGA	O5-C5-C6	2.81	109.93	106.98
2	B	533	FUC	C6-C5-C4	-2.44	109.10	113.06
2	A	532	GAL	O1-C1-O5	-2.18	109.18	111.54
2	B	532	GAL	C1-O5-C5	-2.12	110.60	113.47
2	B	531	NGA	C6-C5-C4	-2.07	108.00	113.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	532	GAL	C3
2	A	531	NGA	C1
2	B	531	NGA	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	284/301 (94%)	0.80	23 (8%) 12 18	20, 20, 20, 20	0
1	B	284/301 (94%)	0.83	18 (6%) 19 28	20, 20, 20, 20	0
All	All	568/602 (94%)	0.81	41 (7%) 16 22	20, 20, 20, 20	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	VAL	5.9
1	B	489	SER	5.8
1	A	487	GLY	5.4
1	B	361	ALA	5.2
1	B	399	ILE	5.1
1	A	510	PHE	4.6
1	A	489	SER	4.6
1	B	231	PHE	4.5
1	A	513	LEU	4.1
1	B	510	PHE	4.0
1	B	230	PRO	3.9
1	B	414	PHE	3.8
1	B	382	PRO	3.8
1	A	467	GLY	3.7
1	B	415	GLY	2.9
1	B	402	ALA	2.8
1	A	414	PHE	2.8
1	A	452	THR	2.7
1	B	400	THR	2.6
1	A	382	PRO	2.6
1	A	468	ARG	2.5
1	A	454	GLY	2.5
1	A	255	ILE	2.4
1	B	490	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	279	THR	2.3
1	A	437	LEU	2.3
1	B	276	LEU	2.3
1	B	284	LEU	2.3
1	A	516	VAL	2.3
1	B	453	VAL	2.3
1	B	370	VAL	2.2
1	A	330	ILE	2.2
1	A	299	ILE	2.2
1	B	341	THR	2.1
1	A	448	GLU	2.1
1	A	260	VAL	2.1
1	A	320	PHE	2.1
1	B	330	ILE	2.1
1	A	399	ILE	2.1
1	A	488	ALA	2.1
1	A	490	SER	2.0

## 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 ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GAL	A	532	11/12	0.18	-	20,20,20,20	0
2	FUC	A	533	11/11	0.16	-	20,20,20,20	0
2	NGA	A	531	14/15	0.15	-	20,20,20,20	0
2	NGA	B	531	14/15	0.21	-	20,20,20,20	0
2	GAL	B	532	11/12	0.21	-	20,20,20,20	0
2	FUC	B	533	11/11	0.36	-	20,20,20,20	0

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.