



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:34 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 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

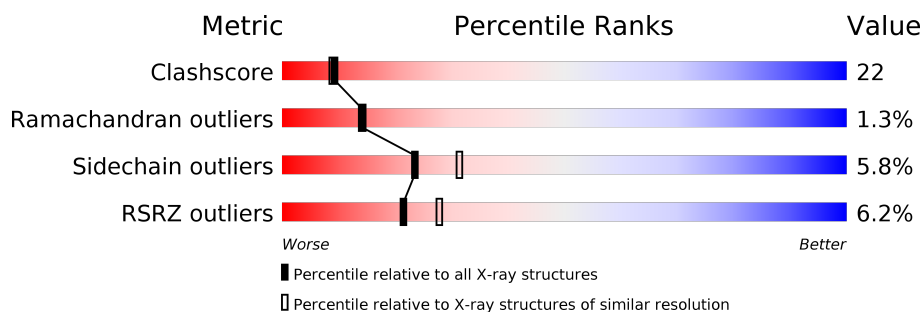
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	301	
1	B	301	

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	NGA	A	531	X	-	-	-
2	GAL	A	532	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NGA	B	531	X	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4540 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 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		

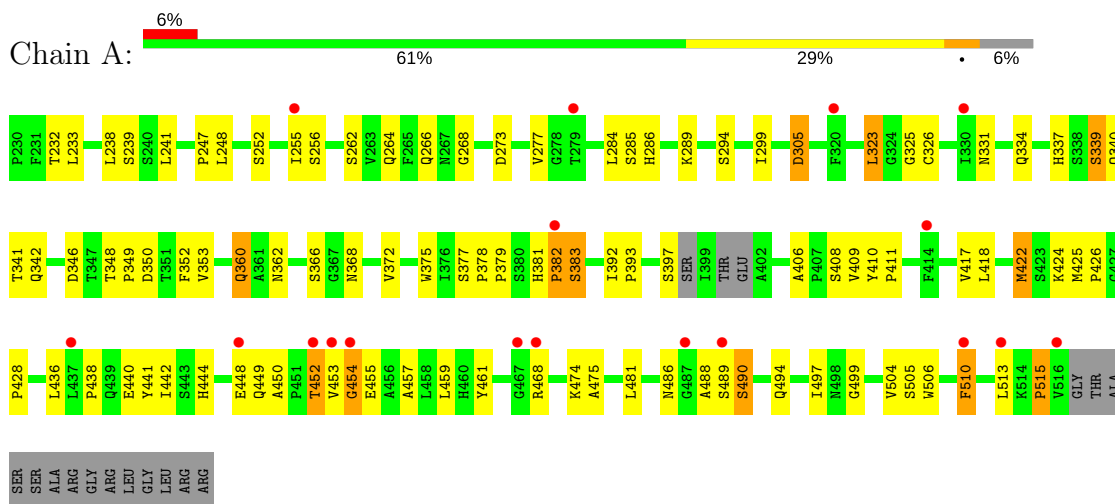
- Molecule 3 is water.

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

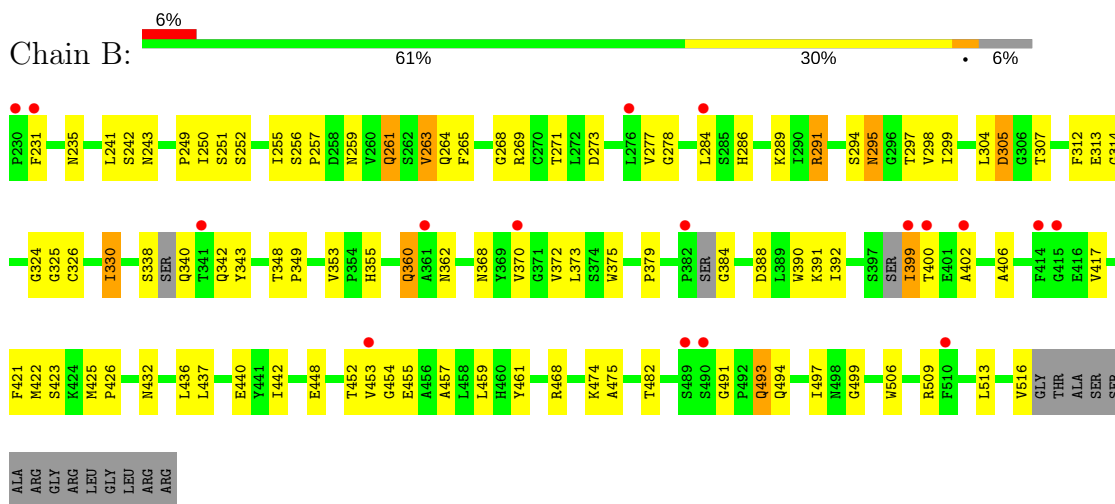
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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 0.244 , (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> )	0.32 , 10.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.084 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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 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	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

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 22.

All (188) 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: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:A:341:THR:HG23	3:A:556:HOH:O	1.89	0.72
1:B:273:ASP:HB2	3:B:583: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	Interatomic distance (Å)	Clash overlap (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:A:360:GLN:NE2	1:A:360:GLN:H	1.97	0.62
1:B:360:GLN:HE21	1:B:360:GLN:H	1.47	0.62
1:B:425:MET:CE	1:B:426:PRO:HD2	2.29	0.62
1:B:291:ARG:HE	1:B:368:ASN:HD21	1.47	0.62
1:B:295:ASN:HD22	1:B:295:ASN:C	2.03	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
1:A:425:MET:HE3	1:A:426:PRO:HD2	1.86	0.58
2:B:531:NGA:H62	3:B:692:HOH:O	2.03	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:294:SER:O	1:A:366:SER:HA	2.04	0.57
1:A:457:ALA:HB2	1:A:506:TRP:CZ3	2.39	0.57
1:B:261:GLN:HA	1:B:261:GLN:NE2	2.09	0.56
1:A:486:ASN:HD21	1:A:515:PRO:HB2	1.71	0.56
1:B:330:ILE:HD11	1:B:343:TYR:CD2	2.41	0.56
1:A:383:SER:HB2	3:A:538:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:SER:HA	1:B:497:ILE:HG22	1.89	0.55
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:323:LEU:N	1:A:323:LEU:HD23	2.23	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:353:VAL:HG11	1:A:397:SER:HB3	1.91	0.52
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: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:504:VAL:O	1:A:505:SER:HB3	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:THR:N	1:A:349:PRO:CD	2.75	0.48
1:B:326:CYS:N	1:B:379:PRO:HG3	2.29	0.48
1:B:330:ILE:HG22	1:B:373:LEU:N	2.28	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:379:PRO:CB	1:A:382:PRO:HD2	2.44	0.47
1:A:453:VAL:HG12	1:A:454:GLY:N	2.25	0.47
1:A:247:PRO:CB	1:A:284:LEU:HD11	2.43	0.47
1:A:334:GLN:HB2	1:A:337:HIS:HB2	1.96	0.47
1:B:314:GLY:O	1:B:355:HIS:HD2	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:255:ILE:HG22	1:B:256:SER:N	2.31	0.45
1:B:375:TRP:HA	1:B:425:MET:HE1	1.98	0.45
1:B:324:GLY:HA2	3:B:628:HOH:O	2.18	0.45
1:A:289:LYS:HE3	1:A:372:VAL:HG22	1.98	0.44
1:A:360:GLN:O	1:A:360:GLN:HG2	2.16	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:A:262:SER:HB3	1:A:410:TYR:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:HG22	1:B:265:PHE:CE2	2.53	0.44
1:B:325:GLY:O	1:B:326:CYS:HB3	2.17	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: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:A:334:GLN:HG2	1:A:368:ASN:O	2.17	0.44
1:B:326:CYS:CA	1:B:379:PRO:HG3	2.47	0.44
1:B:457:ALA:HB2	1:B:506:TRP:CZ3	2.52	0.44
1:B:269:ARG:HA	3:B:587:HOH:O	2.17	0.44
1:B:291:ARG:NH1	1:B:291:ARG:HG3	2.32	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:286:HIS:HD2	3:A:574:HOH:O	2.02	0.43
1:A:425:MET:HE2	1:A:426:PRO:HD2	2.00	0.43
1:A:488:ALA:C	1:A:490:SER:N	2.72	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:A:346:ASP:O	1:A:349:PRO:HD2	2.20	0.42
1:B:257:PRO:HD3	1:B:390:TRP:CE2	2.55	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:377:SER:HB2	1:A:378:PRO:CD	2.50	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: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:A:325:GLY:O	1:A:326:CYS:HB3	2.21	0.40
1:B:257:PRO:HD3	1:B:390:TRP:CZ2	2.56	0.40
1:B:291:ARG:HG2	1:B:370:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:THR:H	1:A:349:PRO:CD	2.34	0.40
1:A:459:LEU:HD11	1:A:475:ALA:HB2	2.03	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 [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	279/301 (93%)	253 (91%)	21 (8%)	5 (2%)	10	9
1	B	276/301 (92%)	261 (95%)	13 (5%)	2 (1%)	25	30
All	All	555/602 (92%)	514 (93%)	34 (6%)	7 (1%)	14	14

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 [i](#)

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%)	31	42
1	B	240/253 (95%)	223 (93%)	17 (7%)	17	22
All	All	480/506 (95%)	452 (94%)	28 (6%)	23	31

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

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

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	14,14,15	0.53	0	15,19,21	1.34	2 (13%)
2	GAL	A	532	2	11,11,12	0.67	0	14,15,17	0.96	1 (7%)
2	FUC	A	533	2	11,11,11	0.56	0	15,16,16	0.71	0
2	NGA	B	531	2	14,14,15	0.52	0	15,19,21	0.95	1 (6%)
2	GAL	B	532	2	11,11,12	0.71	0	14,15,17	0.95	1 (7%)
2	FUC	B	533	2	11,11,11	0.57	0	15,16,16	0.92	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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	531	NGA	C1-O5-C5	-3.50	107.35	112.17
2	A	531	NGA	O5-C1-C2	-2.88	107.46	111.47
2	A	532	GAL	O3-C3-C2	-2.35	104.35	110.02
2	B	533	FUC	C6-C5-C4	-2.23	109.10	113.07
2	B	531	NGA	C6-C5-C4	-2.14	108.00	113.00
2	B	532	GAL	O5-C1-C2	2.02	112.25	110.77

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.



2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	531	NGA	2	0
2	B	533	FUC	1	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	284/301 (94%)	0.66	18 (6%) 21 27	20, 20, 20, 20	0
1	B	284/301 (94%)	0.69	17 (5%) 23 29	20, 20, 20, 20	0
All	All	568/602 (94%)	0.67	35 (6%) 21 28	20, 20, 20, 20	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	VAL	5.7
1	B	489	SER	5.7
1	A	487	GLY	5.1
1	B	399	ILE	5.0
1	B	361	ALA	4.7
1	A	510	PHE	4.5
1	B	231	PHE	4.4
1	A	489	SER	4.4
1	A	513	LEU	4.0
1	B	414	PHE	3.9
1	B	510	PHE	3.8
1	B	230	PRO	3.8
1	B	382	PRO	3.6
1	A	467	GLY	3.4
1	B	415	GLY	2.8
1	B	402	ALA	2.7
1	A	414	PHE	2.7
1	A	452	THR	2.6
1	A	468	ARG	2.5
1	B	400	THR	2.4
1	A	382	PRO	2.4
1	A	454	GLY	2.3
1	A	255	ILE	2.3
1	A	516	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	453	VAL	2.2
1	B	276	LEU	2.2
1	B	284	LEU	2.2
1	B	490	SER	2.2
1	A	437	LEU	2.1
1	A	279	THR	2.1
1	B	341	THR	2.1
1	B	370	VAL	2.1
1	A	330	ILE	2.1
1	A	320	PHE	2.1
1	A	448	GLU	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(Å <sup>2</sup> )	Q<0.9
2	NGA	B	531	14/15	0.81	0.21	2.10	20,20,20,20	0
2	NGA	A	531	14/15	0.85	0.16	-0.36	20,20,20,20	0
2	FUC	A	533	11/11	0.76	0.15	-0.62	20,20,20,20	0
2	GAL	A	532	11/12	0.71	0.18	-	20,20,20,20	0
2	GAL	B	532	11/12	0.75	0.22	-	20,20,20,20	0
2	FUC	B	533	11/11	0.86	0.35	-	20,20,20,20	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.