



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 PM GMT

PDB ID : 4GDJ
Title : A subtype N10 neuraminidase-like protein of A/little yellow-shouldered bat/
Guatemala/060/2010
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2012-07-31
Resolution : 2.00 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

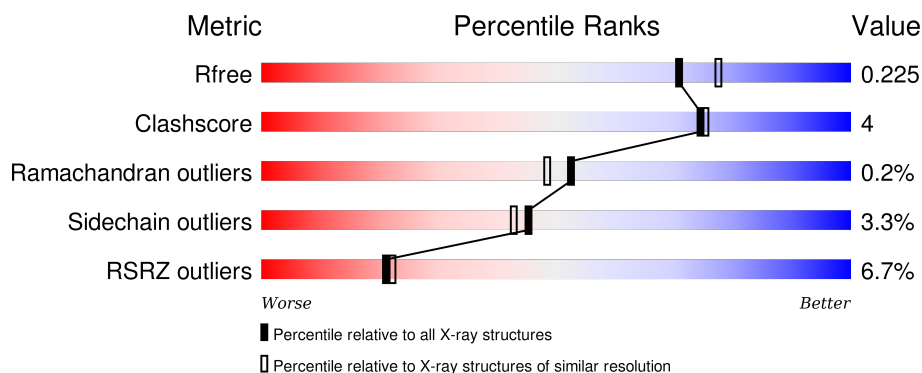
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	373	<div> <div>5%</div> <div>78%</div> <div>6%</div> <div>15%</div> </div>
1	B	373	<div> <div>6%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	C	373	<div> <div>6%</div> <div>74%</div> <div>9%</div> <div>16%</div> </div>
1	D	373	<div> <div>5%</div> <div>75%</div> <div>8%</div> <div>16%</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 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20514 atoms, of which 9599 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	317	Total	C	H	N	O	S	0	0	0
			4874	1560	2396	421	479	18			
1	B	321	Total	C	H	N	O	S	0	0	0
			4942	1579	2435	426	484	18			
1	C	314	Total	C	H	N	O	S	0	0	0
			4839	1546	2383	418	474	18			
1	D	314	Total	C	H	N	O	S	0	0	0
			4841	1547	2385	418	474	17			

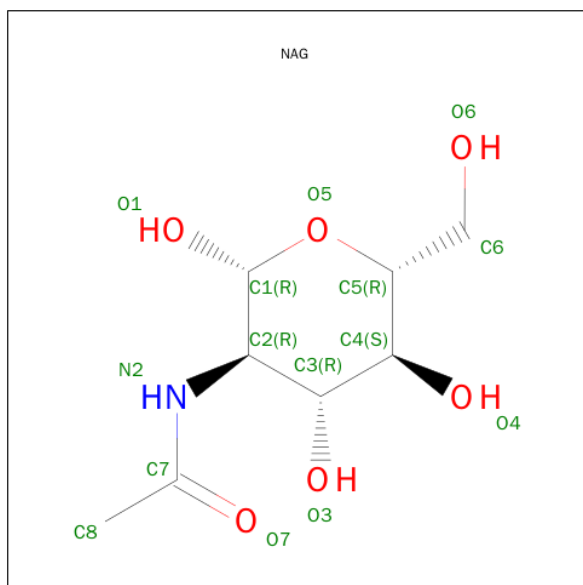
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	EXPRESSION TAG	UNP H6QM95
A	78	SER	-	EXPRESSION TAG	UNP H6QM95
A	79	PRO	-	EXPRESSION TAG	UNP H6QM95
A	80	SER	-	EXPRESSION TAG	UNP H6QM95
A	81	ARG	-	EXPRESSION TAG	UNP H6QM95
B	77	GLY	-	EXPRESSION TAG	UNP H6QM95
B	78	SER	-	EXPRESSION TAG	UNP H6QM95
B	79	PRO	-	EXPRESSION TAG	UNP H6QM95
B	80	SER	-	EXPRESSION TAG	UNP H6QM95
B	81	ARG	-	EXPRESSION TAG	UNP H6QM95
C	77	GLY	-	EXPRESSION TAG	UNP H6QM95
C	78	SER	-	EXPRESSION TAG	UNP H6QM95
C	79	PRO	-	EXPRESSION TAG	UNP H6QM95
C	80	SER	-	EXPRESSION TAG	UNP H6QM95
C	81	ARG	-	EXPRESSION TAG	UNP H6QM95
D	77	GLY	-	EXPRESSION TAG	UNP H6QM95
D	78	SER	-	EXPRESSION TAG	UNP H6QM95
D	79	PRO	-	EXPRESSION TAG	UNP H6QM95
D	80	SER	-	EXPRESSION TAG	UNP H6QM95
D	81	ARG	-	EXPRESSION TAG	UNP H6QM95

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			48	28	2	18		
2	B	4	Total	C	N	O	0	0
			48	28	2	18		
2	C	4	Total	C	N	O	0	0
			48	28	2	18		
2	D	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

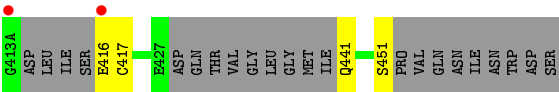
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

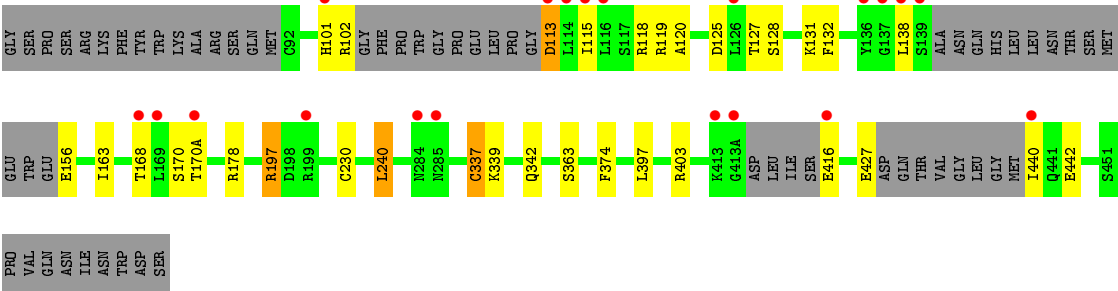
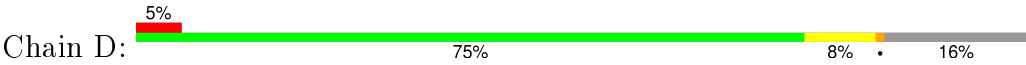
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	189	Total 189	O 189	0	0
5	B	195	Total 195	O 195	0	0
5	C	180	Total 180	O 180	0	0
5	D	174	Total 174	O 174	0	0

- Molecule 1: Neuraminidase





● Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 107.90Å 345.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.00 48.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.85-2.00) 97.7 (48.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.2_869)	Depositor
R, R_{free}	0.189 , 0.226 0.193 , 0.225	Depositor DCC
R_{free} test set	6812 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	7 of 135469 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20514	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, CA, FUL, 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	0.64	0/2527	0.78	4/3413 (0.1%)
1	B	0.62	0/2558	0.75	2/3456 (0.1%)
1	C	0.60	0/2505	0.78	3/3383 (0.1%)
1	D	0.59	0/2505	0.74	1/3384 (0.0%)
All	All	0.61	0/10095	0.76	10/13636 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	CYS	CA-CB-SG	11.11	133.99	114.00
1	A	118	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	C	197	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	D	240	LEU	CA-CB-CG	-5.63	102.35	115.30
1	B	138	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	C	178	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	240	LEU	CA-CB-CG	-5.22	103.29	115.30
1	A	118	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	240	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	C	327	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2478	2396	2403	16	0
1	B	2507	2435	2433	16	0
1	C	2456	2383	2382	29	0
1	D	2456	2385	2384	22	0
2	A	48	0	43	0	0
2	B	48	0	43	1	0
2	C	48	0	43	0	0
2	D	48	0	43	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	189	0	0	3	0
5	B	195	0	0	2	0
5	C	180	0	0	5	0
5	D	174	0	0	2	0
All	All	10915	9599	9852	81	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 4.

All (81) 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:178:ARG:NH1	5:B:707:HOH:O	1.59	1.32
1:A:118:ARG:NH2	1:A:156:GLU:OE2	1.97	0.96
1:C:178:ARG:CZ	1:C:197:ARG:HH12	1.79	0.96
1:B:336:SER:OG	1:B:339:LYS:HG2	1.69	0.93
1:C:306:THR:HG23	1:C:309:ASP:OD1	1.73	0.88
1:D:118:ARG:NH2	1:D:156:GLU:OE2	2.14	0.80
1:C:371:GLN:HB2	1:C:403:ARG:HD3	1.64	0.79
1:C:210:GLU:OE2	5:C:715:HOH:O	2.02	0.76
1:D:337:CYS:SG	5:D:663:HOH:O	2.43	0.76
1:B:451:SER:OG	1:B:452:PRO:HD3	1.85	0.76
1:B:451:SER:OG	1:B:452:PRO:CD	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ARG:CZ	1:C:197:ARG:NH1	2.55	0.69
1:A:249:GLN:HG3	5:A:763:HOH:O	1.94	0.67
1:C:178:ARG:NH2	1:C:197:ARG:HH12	1.92	0.67
1:C:286:LEU:HD23	1:C:288:LYS:NZ	2.09	0.67
1:A:451:SER:O	1:A:451:SER:OG	2.07	0.66
1:C:327:ARG:O	1:C:344:LYS:HE3	1.95	0.65
1:C:93:GLU:HB2	1:C:359:PRO:HD2	1.78	0.64
1:A:427:GLU:N	1:A:427:GLU:OE1	2.31	0.64
1:B:271:THR:OG1	2:B:501:NAG:H5	1.98	0.63
1:D:118:ARG:HH21	1:D:156:GLU:CD	2.03	0.61
1:D:131:LYS:HG3	1:D:163:ILE:HD12	1.84	0.58
1:A:118:ARG:NH2	1:A:156:GLU:CD	2.56	0.57
1:A:152:GLU:OE2	1:A:152:GLU:HA	2.04	0.57
1:C:286:LEU:HD23	1:C:288:LYS:HZ2	1.69	0.57
1:A:403:ARG:O	1:A:427:GLU:OE1	2.22	0.57
1:B:194:SER:OG	5:B:707:HOH:O	2.18	0.55
1:C:210:GLU:CD	5:C:715:HOH:O	2.44	0.54
1:D:197:ARG:HE	1:D:197:ARG:CA	2.18	0.54
1:C:93:GLU:HG2	1:C:451:SER:O	2.08	0.54
1:C:118:ARG:NH1	1:C:119:ARG:HD2	2.23	0.53
1:D:403:ARG:HD3	1:D:427:GLU:CD	2.28	0.53
1:C:288:LYS:CD	1:C:304:ARG:HG2	2.39	0.53
1:C:441:GLN:OE1	1:C:441:GLN:HA	2.07	0.53
1:A:245:PRO:HD2	5:A:763:HOH:O	2.09	0.52
1:A:352:PHE:HB2	1:A:409:PHE:CE2	2.44	0.52
1:D:113:ASP:OD1	1:D:113:ASP:N	2.43	0.52
1:C:93:GLU:HB2	1:C:359:PRO:CD	2.41	0.51
1:B:114:LEU:O	1:B:138:LEU:HD12	2.10	0.51
1:D:440:ILE:HD11	1:D:442:GLU:OE2	2.11	0.51
1:D:440:ILE:CD1	1:D:442:GLU:OE2	2.59	0.51
1:C:416:GLU:N	5:C:745:HOH:O	2.44	0.50
1:D:168:THR:HG22	1:D:170(A):THR:OG1	2.12	0.49
1:C:306:THR:CG2	1:C:309:ASP:OD1	2.54	0.49
1:D:118:ARG:NH1	1:D:119:ARG:HD2	2.28	0.49
1:B:209:GLU:CD	1:B:209:GLU:H	2.16	0.49
1:C:91:MET:HG2	1:C:92:CYS:H	1.78	0.48
1:A:393:LEU:HD13	1:D:397:LEU:CD2	2.43	0.48
1:B:269:ASN:OD1	1:B:271:THR:HG23	2.14	0.48
1:C:219:ARG:HG3	1:C:251:VAL:HG21	1.95	0.47
1:C:248:ASN:OD1	1:C:249:GLN:HG3	2.14	0.47
1:C:288:LYS:HE3	1:C:304:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HA	1:D:197:ARG:HE	1.78	0.46
1:D:120:ALA:HA	1:D:132:PHE:O	2.16	0.46
1:B:120:ALA:HA	1:B:132:PHE:O	2.16	0.46
1:B:209:GLU:N	1:B:209:GLU:CD	2.69	0.46
1:C:199:ARG:NH1	5:C:697:HOH:O	2.49	0.46
1:C:173:MET:HE1	5:C:743:HOH:O	2.16	0.45
1:B:113:ASP:N	1:B:113:ASP:OD1	2.46	0.45
1:C:327:ARG:O	1:C:344:LYS:CE	2.65	0.43
1:B:363:SER:HA	1:B:375:VAL:O	2.19	0.43
1:B:352:PHE:HB2	1:B:409:PHE:CE2	2.54	0.43
1:A:363:SER:HA	1:A:375:VAL:O	2.19	0.43
1:B:361:TRP:HA	1:B:377:GLU:O	2.18	0.42
1:D:115:ILE:HG13	1:D:168:THR:HA	2.00	0.42
1:C:286:LEU:CD2	1:C:288:LYS:HZ2	2.33	0.42
1:B:234:GLU:OE1	1:B:307:LYS:NZ	2.41	0.42
1:D:363:SER:HB2	1:D:374:PHE:CZ	2.54	0.42
1:C:327:ARG:C	1:C:344:LYS:HE3	2.39	0.42
1:D:156:GLU:OE1	1:D:178:ARG:HG2	2.20	0.42
1:D:403:ARG:HD3	1:D:427:GLU:OE2	2.21	0.41
1:C:352:PHE:HB2	1:C:409:PHE:CE2	2.55	0.41
1:C:178:ARG:NH2	1:C:197:ARG:NH1	2.63	0.41
1:A:114:LEU:HD12	1:A:168:THR:HG22	2.03	0.41
1:D:339:LYS:HE3	5:D:721:HOH:O	2.20	0.41
1:A:371:GLN:OE1	1:A:403:ARG:NH2	2.54	0.41
1:D:197:ARG:HA	1:D:197:ARG:NE	2.36	0.41
1:A:253:ARG:HG2	1:A:267:GLN:HA	2.03	0.41
1:D:125:ASP:OD1	1:D:128:SER:N	2.50	0.41
1:A:393:LEU:HD13	1:D:397:LEU:HD23	2.03	0.40
1:A:249:GLN:CD	5:A:738:HOH:O	2.60	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	307/373 (82%)	294 (96%)	12 (4%)	1 (0%)	46	41
1	B	311/373 (83%)	300 (96%)	10 (3%)	1 (0%)	46	41
1	C	304/373 (82%)	294 (97%)	10 (3%)	0	100	100
1	D	304/373 (82%)	292 (96%)	12 (4%)	0	100	100
All	All	1226/1492 (82%)	1180 (96%)	44 (4%)	2 (0%)	52	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	B	112	GLY

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	279/328 (85%)	270 (97%)	9 (3%)	46	44
1	B	283/328 (86%)	276 (98%)	7 (2%)	55	55
1	C	277/328 (84%)	268 (97%)	9 (3%)	46	44
1	D	277/328 (84%)	265 (96%)	12 (4%)	35	30
All	All	1116/1312 (85%)	1079 (97%)	37 (3%)	45	43

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER
1	A	152	GLU
1	A	170	SER
1	A	240	LEU
1	A	266	LYS
1	A	307	LYS
1	A	337	CYS
1	A	416	GLU
1	A	451	SER

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	152	GLU
1	B	230	CYS
1	B	240	LEU
1	B	342	GLN
1	B	419	ARG
1	B	427	GLU
1	C	102	ARG
1	C	114	LEU
1	C	127	THR
1	C	240	LEU
1	C	266	LYS
1	C	342	GLN
1	C	387	GLU
1	C	403	ARG
1	C	417	CYS
1	D	101	HIS
1	D	102	ARG
1	D	113	ASP
1	D	127	THR
1	D	138	LEU
1	D	170	SER
1	D	197	ARG
1	D	230	CYS
1	D	240	LEU
1	D	337	CYS
1	D	342	GLN
1	D	416	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	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 ⓘ

16 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	NAG	A	501	1,2	14,14,15	0.78	0	15,19,21	1.20	1 (6%)
2	NAG	A	502	2	14,14,15	0.45	0	15,19,21	1.02	0
2	FUC	A	503	2	10,10,11	0.74	0	14,14,16	1.26	2 (14%)
2	FUL	A	504	2	10,10,11	0.91	0	14,14,16	4.41	5 (35%)
2	NAG	B	501	1,2	14,14,15	0.71	0	15,19,21	1.10	1 (6%)
2	NAG	B	502	2	14,14,15	0.64	0	15,19,21	0.86	0
2	FUC	B	503	2	10,10,11	0.78	0	14,14,16	1.25	2 (14%)
2	FUL	B	504	2	10,10,11	0.89	0	14,14,16	4.31	7 (50%)
2	NAG	C	501	1,2	14,14,15	0.56	0	15,19,21	1.45	3 (20%)
2	NAG	C	502	2	14,14,15	0.56	0	15,19,21	1.40	4 (26%)
2	FUC	C	503	2	10,10,11	0.80	0	14,14,16	1.58	4 (28%)
2	FUL	C	504	2	10,10,11	0.81	0	14,14,16	4.97	9 (64%)
2	NAG	D	501	1,2	14,14,15	0.67	0	15,19,21	1.07	1 (6%)
2	NAG	D	502	2	14,14,15	0.56	0	15,19,21	1.30	1 (6%)
2	FUC	D	503	2	10,10,11	0.65	0	14,14,16	1.08	1 (7%)
2	FUL	D	504	2	10,10,11	0.78	0	14,14,16	2.10	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	502	2	-	0/6/23/26	0/1/1/1
2	FUC	A	503	2	-	0/0/17/20	0/1/1/1
2	FUL	A	504	2	-	0/0/17/20	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	FUC	B	503	2	-	0/0/17/20	0/1/1/1
2	FUL	B	504	2	-	0/0/17/20	0/1/1/1
2	NAG	C	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	502	2	-	0/6/23/26	0/1/1/1
2	FUC	C	503	2	-	0/0/17/20	0/1/1/1
2	FUL	C	504	2	-	0/0/17/20	0/1/1/1
2	NAG	D	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	502	2	-	0/6/23/26	0/1/1/1
2	FUC	D	503	2	-	0/0/17/20	0/1/1/1
2	FUL	D	504	2	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	504	FUL	C1-O5-C5	-13.33	91.79	112.38
2	B	504	FUL	C1-C2-C3	-12.82	94.38	109.54
2	A	504	FUL	C1-C2-C3	-12.68	94.54	109.54
2	C	504	FUL	C1-C2-C3	-10.59	97.02	109.54
2	A	504	FUL	C1-O5-C5	-8.85	98.72	112.38
2	B	504	FUL	C1-O5-C5	-6.71	102.02	112.38
2	D	504	FUL	C1-C2-C3	-4.96	103.68	109.54
2	D	504	FUL	O5-C1-C2	-4.09	104.22	110.86
2	C	504	FUL	C2-C3-C4	-3.78	104.63	111.04
2	C	501	NAG	O3-C3-C2	-3.74	101.71	109.11
2	A	501	NAG	O3-C3-C2	-3.65	101.88	109.11
2	B	504	FUL	O5-C1-C2	-3.25	105.59	110.86
2	D	501	NAG	C2-N2-C7	-2.89	119.32	123.04
2	B	504	FUL	C2-C3-C4	-2.72	106.43	111.04
2	D	504	FUL	C1-O5-C5	-2.64	108.30	112.38
2	C	503	FUC	O2-C2-C1	-2.51	104.18	109.21
2	D	503	FUC	O2-C2-C1	-2.44	104.31	109.21
2	C	503	FUC	C6-C5-C4	-2.37	108.42	113.08
2	B	503	FUC	O5-C1-C2	-2.35	107.04	110.86
2	B	503	FUC	O2-C2-C3	-2.30	105.48	110.12
2	C	502	NAG	C6-C5-C4	-2.25	107.46	113.02
2	C	504	FUL	O5-C1-C2	-2.25	107.21	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	FUC	O2-C2-C3	-2.23	105.63	110.12
2	A	503	FUC	O5-C1-C2	-2.12	107.41	110.86
2	C	504	FUL	O4-C4-C3	-2.04	105.75	110.34
2	C	501	NAG	C3-C2-N2	-2.02	105.71	110.56
2	C	504	FUL	C3-C4-C5	2.03	113.14	109.72
2	C	502	NAG	O5-C5-C6	2.12	111.94	107.35
2	D	504	FUL	O2-C2-C1	2.23	113.68	109.21
2	B	504	FUL	O5-C5-C6	2.28	109.90	106.13
2	C	502	NAG	C3-C4-C5	2.42	114.41	110.20
2	C	501	NAG	C1-O5-C5	2.43	115.33	112.25
2	B	504	FUL	C3-C4-C5	2.49	113.92	109.72
2	C	504	FUL	O2-C2-C1	2.55	114.31	109.21
2	B	501	NAG	C1-O5-C5	2.56	115.49	112.25
2	C	502	NAG	C1-O5-C5	2.56	115.50	112.25
2	A	504	FUL	O2-C2-C1	2.58	114.38	109.21
2	A	503	FUC	O5-C5-C6	2.62	110.47	106.13
2	C	503	FUC	O5-C5-C6	2.68	110.56	106.13
2	A	504	FUL	O5-C5-C6	2.78	110.73	106.13
2	C	504	FUL	O2-C2-C3	2.81	115.77	110.12
2	A	504	FUL	C3-C4-C5	3.08	114.91	109.72
2	C	504	FUL	O5-C5-C6	3.30	111.59	106.13
2	B	504	FUL	O2-C2-C3	3.65	117.47	110.12
2	D	502	NAG	C1-O5-C5	3.71	116.96	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAG	1	0

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	NAG	A	505	1	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
3	NAG	A	506	1	14,14,15	0.43	0	15,19,21	0.71	0
3	NAG	B	505	1	14,14,15	0.54	0	15,19,21	0.76	0
3	NAG	B	506	1	14,14,15	0.51	0	15,19,21	1.02	1 (6%)
3	NAG	C	505	1	14,14,15	0.40	0	15,19,21	1.50	2 (13%)
3	NAG	D	505	1	14,14,15	0.53	0	15,19,21	0.79	0

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	505	1	-	0/6/23/26	0/1/1/1
3	NAG	A	506	1	-	0/6/23/26	0/1/1/1
3	NAG	B	505	1	-	0/6/23/26	0/1/1/1
3	NAG	B	506	1	-	0/6/23/26	0/1/1/1
3	NAG	C	505	1	-	0/6/23/26	0/1/1/1
3	NAG	D	505	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	NAG	C1-O5-C5	-3.72	107.53	112.25
3	C	505	NAG	C2-N2-C7	-2.03	120.44	123.04
3	B	506	NAG	C1-O5-C5	3.10	116.18	112.25
3	C	505	NAG	C1-O5-C5	4.74	118.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	317/373 (84%)	0.31	20 (6%) 23 24	19, 30, 63, 96	0
1	B	321/373 (86%)	0.34	21 (6%) 22 23	19, 30, 67, 108	0
1	C	314/373 (84%)	0.29	24 (7%) 17 18	20, 33, 68, 101	0
1	D	314/373 (84%)	0.37	20 (6%) 23 24	21, 33, 69, 103	0
All	All	1266/1492 (84%)	0.33	85 (6%) 21 22	19, 31, 68, 108	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	LEU	8.9
1	A	440	ILE	7.6
1	D	413(A)	GLY	7.6
1	B	111	PRO	7.6
1	D	114	LEU	6.8
1	C	114	LEU	6.7
1	C	138	LEU	6.6
1	A	140	ALA	6.6
1	D	139	SER	6.3
1	B	139	SER	5.7
1	C	139	SER	5.7
1	B	138	LEU	5.4
1	B	114	LEU	5.3
1	C	137	GLY	5.0
1	B	452	PRO	5.0
1	D	169	LEU	4.7
1	D	136	TYR	4.7
1	A	113	ASP	4.7
1	D	116	LEU	4.6
1	B	113	ASP	4.6
1	C	169	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	4.6
1	C	170(A)	THR	4.5
1	B	91	MET	4.3
1	D	199	ARG	4.2
1	B	112	GLY	4.2
1	A	114	LEU	4.1
1	A	416	GLU	4.1
1	D	137	GLY	4.0
1	B	116	LEU	4.0
1	C	113	ASP	3.9
1	A	91	MET	3.9
1	A	169	LEU	3.9
1	C	136	TYR	3.8
1	A	139	SER	3.8
1	C	168	THR	3.7
1	C	170	SER	3.7
1	A	137	GLY	3.6
1	C	127	THR	3.6
1	B	199	ARG	3.6
1	A	127	THR	3.5
1	D	285	ASN	3.5
1	C	285	ASN	3.5
1	D	115	ILE	3.5
1	B	440	ILE	3.4
1	C	91	MET	3.4
1	D	113	ASP	3.4
1	C	115	ILE	3.4
1	D	440	ILE	3.4
1	B	413(A)	GLY	3.2
1	C	102	ARG	3.1
1	C	401	ASN	3.1
1	D	168	THR	3.1
1	C	166	ALA	3.0
1	C	416	GLU	3.0
1	D	416	GLU	2.9
1	C	116	LEU	2.9
1	D	284	ASN	2.7
1	B	137	GLY	2.7
1	B	169	LEU	2.7
1	D	126	LEU	2.7
1	A	116	LEU	2.6
1	D	101	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	164	GLY	2.5
1	B	337	CYS	2.5
1	C	284	ASN	2.5
1	A	170(A)	THR	2.5
1	D	170(A)	THR	2.4
1	A	339	LYS	2.4
1	A	136	TYR	2.4
1	B	342	GLN	2.4
1	A	413(A)	GLY	2.4
1	A	101	HIS	2.4
1	B	339	LYS	2.4
1	B	170	SER	2.3
1	C	286	LEU	2.3
1	A	199	ARG	2.3
1	B	166	ALA	2.3
1	A	170	SER	2.2
1	D	413	LYS	2.1
1	C	171	SER	2.1
1	C	283	ILE	2.1
1	C	413(A)	GLY	2.0
1	A	166	ALA	2.0
1	B	165	SER	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(Å ²)	Q<0.9
2	NAG	C	501	14/15	0.94	0.12	2.33	31,36,46,48	0
2	NAG	D	501	14/15	0.94	0.13	0.97	33,46,52,57	0
2	FUC	D	503	10/11	0.96	0.11	-0.03	33,36,43,45	0
2	FUC	A	503	10/11	0.96	0.10	-0.52	35,41,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FUC	C	503	10/11	0.97	0.08	-0.71	32,36,39,41	0
2	FUC	B	503	10/11	0.96	0.08	-1.79	29,36,44,51	0
2	NAG	D	502	14/15	0.94	0.21	-	53,60,75,88	0
2	NAG	B	501	14/15	0.92	0.14	-	26,42,46,49	0
2	FUL	A	504	10/11	0.90	0.12	-	43,50,53,55	0
2	FUL	C	504	10/11	0.92	0.13	-	36,43,57,58	0
2	FUL	D	504	10/11	0.88	0.22	-	47,56,79,92	0
2	NAG	A	502	14/15	0.93	0.17	-	28,49,62,87	0
2	NAG	B	502	14/15	0.92	0.17	-	41,57,69,84	0
2	NAG	C	502	14/15	0.91	0.16	-	47,57,73,83	0
2	FUL	B	504	10/11	0.88	0.18	-	42,52,62,66	0
2	NAG	A	501	14/15	0.94	0.10	-	32,39,48,48	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
4	CA	D	506	1/1	0.99	0.12	0.76	24,24,24,24	0
4	CA	A	507	1/1	1.00	0.10	-0.63	23,23,23,23	0
4	CA	B	507	1/1	1.00	0.09	-0.83	22,22,22,22	0
4	CA	C	506	1/1	0.99	0.07	-1.41	25,25,25,25	0
3	NAG	B	505	14/15	0.86	0.34	-	76,88,100,117	0
3	NAG	C	505	14/15	0.83	0.29	-	73,84,92,102	0
3	NAG	B	506	14/15	0.69	0.35	-	72,85,96,99	0
3	NAG	D	505	14/15	0.69	0.30	-	67,81,86,90	0
3	NAG	A	506	14/15	0.80	0.21	-	71,84,95,103	0
3	NAG	A	505	14/15	0.80	0.36	-	68,86,96,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.