



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:41 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 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/ValidationPDFNotes.html>

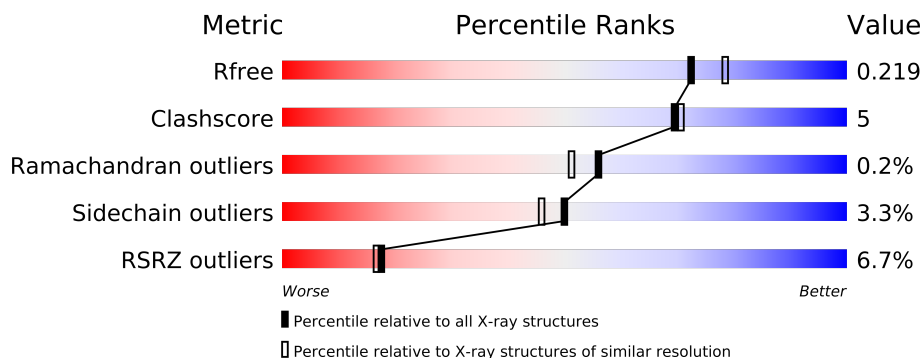
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. 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	373	
1	B	373	
1	C	373	
1	D	373	

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 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 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		

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 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

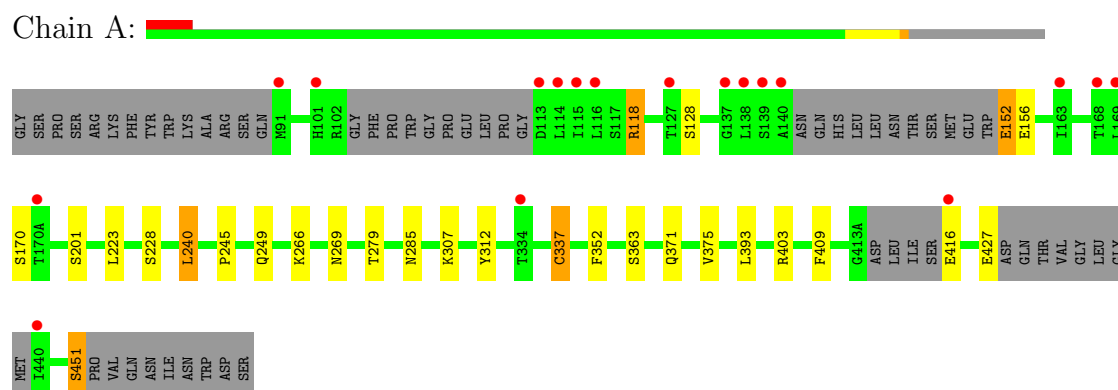
- Molecule 5 is water.

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

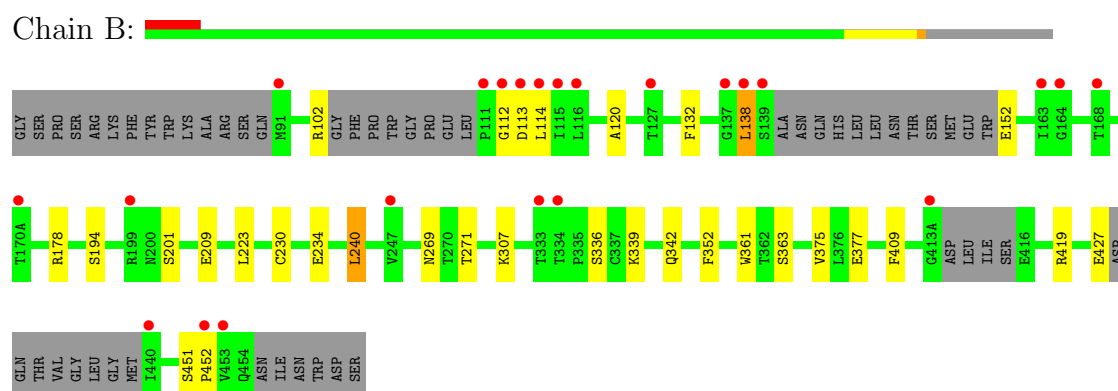
3 Residue-property plots

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.

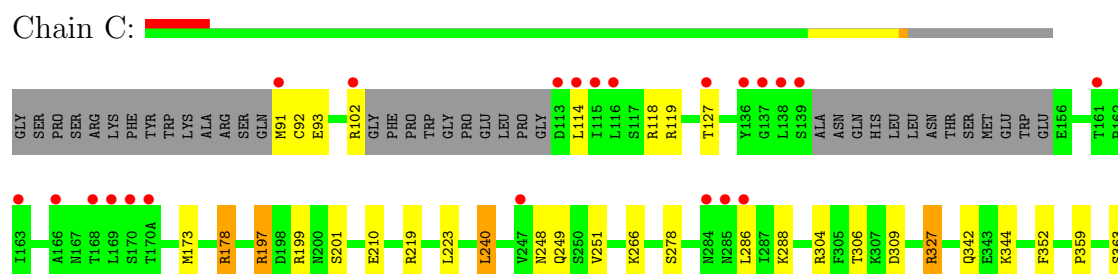
• Molecule 1: Neuraminidase

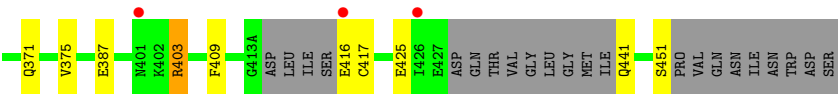


• Molecule 1: Neuraminidase



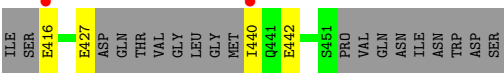
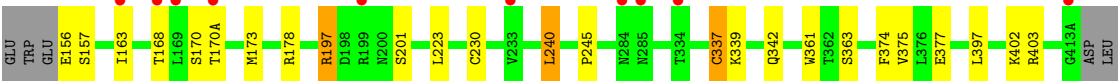
• Molecule 1: Neuraminidase





● Molecule 1: Neuraminidase

Chain D:



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 0.183 , 0.219	Depositor DCC
R_{free} test set	6775 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.

5 Model quality

5.1 Standard geometry

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 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	2478	2396	5	17	0
1	B	2507	2435	0	16	0
1	C	2456	2383	0	33	0
1	D	2456	2385	0	27	0
2	A	48	0	0	0	0
2	B	48	0	0	0	0
2	C	48	0	0	0	0
2	D	48	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	14	0	0	0	0
3	D	14	0	0	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	3	0
All	All	10915	9599	5	92	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 5.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	0.95
1:B:336:SER:OG	1:B:339:LYS:HG2	1.69	0.92
1:A:228:SER:HG	1:A:279:THR:HG1	1.20	0.87
1:C:306:THR:HG21	1:C:309:ASP:OD1	1.73	0.87
1:D:118:ARG:NH2	1:D:156:GLU:OE2	2.14	0.80
1:C:371:GLN:HB2	1:C:403:ARG:HD3	1.66	0.77
1:C:210:GLU:OE2	5:C:715:HOH:O	2.02	0.76
1:C:201:SER:HG	1:C:223:LEU:H	1.30	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	1.88	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:SER:HG	1:A:223:LEU:H	1.35	0.73
1:A:269:ASN:H	1:A:312:TYR:HH	1.40	0.69
1:B:451:SER:OG	1:B:452:PRO:CD	2.39	0.69
1:C:178:ARG:CZ	1:C:197:ARG:NH1	2.55	0.69
1:A:249:GLN:HG3	5:A:763:HOH:O	1.93	0.67
1:C:327:ARG:O	1:C:344:LYS:HE3	1.94	0.67
1:C:178:ARG:NH2	1:C:197:ARG:HH12	1.93	0.66
1:C:286:LEU:HD21	1:C:288:LYS:NZ	2.10	0.66
1:A:451:SER:O	1:A:451:SER:OG	2.07	0.66
1:D:157:SER:OG	1:D:173:MET:HE3	1.97	0.65
1:A:427:GLU:N	1:A:427:GLU:OE1	2.31	0.64
1:D:118:ARG:HH21	1:D:156:GLU:CD	2.03	0.61
1:C:286:LEU:HD21	1:C:288:LYS:HZ3	1.66	0.61
1:C:93:GLU:HB2	1:C:359:PRO:HD2	1.82	0.61
1:A:152:GLU:OE2	1:A:152:GLU:HA	2.02	0.59
1:C:441:GLN:HA	1:C:441:GLN:OE1	2.01	0.59
1:A:118:ARG:NH2	1:A:156:GLU:CD	2.56	0.57
1:A:403:ARG:O	1:A:427:GLU:OE1	2.22	0.57
1:D:197:ARG:HA	1:D:197:ARG:HE	1.68	0.56
1:C:118:ARG:NH1	1:C:119:ARG:HD2	2.20	0.56
1:D:131:LYS:HG3	1:D:163:ILE:HD12	1.87	0.56
1:C:201:SER:HG	1:C:223:LEU:N	2.01	0.56
1:A:201:SER:HG	1:A:223:LEU:N	2.03	0.56
1:B:194:SER:OG	5:B:707:HOH:O	2.18	0.55
1:C:286:LEU:CD2	1:C:288:LYS:HZ3	2.20	0.55
1:A:245:PRO:HD2	5:A:763:HOH:O	2.06	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:D:403:ARG:HD3	1:D:427:GLU:CD	2.28	0.54
1:C:288:LYS:CD	1:C:304:ARG:HG2	2.39	0.53
1:B:234:GLU:OE1	1:B:307:LYS:NZ	2.41	0.53
1:D:113:ASP:OD1	1:D:113:ASP:N	2.43	0.52
1:B:201:SER:HG	1:B:223:LEU:H	1.57	0.52
1:D:118:ARG:NH1	1:D:119:ARG:HD2	2.26	0.51
1:A:352:PHE:HB2	1:A:409:PHE:CE2	2.45	0.51
1:C:93:GLU:HG2	1:C:451:SER:O	2.10	0.51
1:D:197:ARG:HA	1:D:197:ARG:NE	2.25	0.51
1:D:440:ILE:CD1	1:D:442:GLU:OE2	2.59	0.51
1:C:93:GLU:HB2	1:C:359:PRO:CD	2.41	0.51
1:C:288:LYS:HE3	1:C:304:ARG:HG2	1.94	0.50
1:D:440:ILE:HD11	1:D:442:GLU:OE2	2.12	0.50
1:B:114:LEU:O	1:B:138:LEU:HD11	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:416:GLU:N	5:C:745:HOH:O	2.44	0.50
1:D:201:SER:HG	1:D:223:LEU:H	1.60	0.49
1:C:306:THR:CG2	1:C:309:ASP:OD1	2.54	0.49
1:C:91:MET:HG2	1:C:92:CYS:H	1.78	0.49
1:B:209:GLU:CD	1:B:209:GLU:H	2.16	0.49
1:D:168:THR:HG23	1:D:170(A):THR:OG1	2.13	0.49
1:B:120:ALA:HA	1:B:132:PHE:O	2.14	0.48
1:D:120:ALA:HA	1:D:132:PHE:O	2.14	0.48
1:C:248:ASN:OD1	1:C:249:GLN:HG3	2.14	0.48
1:C:240:LEU:HD22	1:C:278:SER:HG	1.79	0.48
1:A:393:LEU:HD13	1:D:397:LEU:CD2	2.44	0.47
1:B:269:ASN:OD1	1:B:271:THR:HG23	2.15	0.47
1:C:219:ARG:HG3	1:C:251:VAL:HG21	1.96	0.46
1:B:361:TRP:HA	1:B:377:GLU:O	2.15	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:B:113:ASP:N	1:B:113:ASP:OD1	2.46	0.45
1:C:173:MET:HE1	5:C:743:HOH:O	2.16	0.44
1:B:363:SER:HA	1:B:375:VAL:O	2.18	0.44
1:D:115:ILE:HG13	1:D:168:THR:HA	1.99	0.44
1:D:363:SER:HB2	1:D:374:PHE:CZ	2.53	0.43
1:A:363:SER:HA	1:A:375:VAL:O	2.19	0.43
1:C:327:ARG:C	1:C:344:LYS:HE3	2.39	0.43
1:B:352:PHE:HB2	1:B:409:PHE:CE2	2.55	0.42
1:D:403:ARG:HD3	1:D:427:GLU:OE2	2.20	0.42
1:D:245:PRO:HD2	5:D:708:HOH:O	2.20	0.42
1:C:363:SER:HA	1:C:375:VAL:O	2.20	0.41
1:D:363:SER:HA	1:D:375:VAL:O	2.20	0.41
1:D:402:LYS:HD2	1:D:402:LYS:HA	1.84	0.41
1:C:178:ARG:NH2	1:C:197:ARG:NH1	2.63	0.41
1:D:156:GLU:OE1	1:D:178:ARG:HG2	2.20	0.41
1:D:361:TRP:HA	1:D:377:GLU:O	2.20	0.41
1:A:371:GLN:OE1	1:A:403:ARG:NH2	2.54	0.41
1:D:125:ASP:OD1	1:D:128:SER:N	2.50	0.41
1:D:339:LYS:HE3	5:D:721:HOH:O	2.20	0.41
1:C:352:PHE:HB2	1:C:409:PHE:CE2	2.55	0.40
1:C:425:GLU:HB3	1:C:441:GLN:OE1	2.21	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%)	50	44
1	B	311/373 (83%)	300 (96%)	10 (3%)	1 (0%)	50	44
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%)	56	51

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%)	51	47
1	B	283/328 (86%)	276 (98%)	7 (2%)	60	59
1	C	277/328 (84%)	268 (97%)	9 (3%)	51	47
1	D	277/328 (84%)	265 (96%)	12 (4%)	40	33
All	All	1116/1312 (85%)	1079 (97%)	37 (3%)	50	46

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

Mol	Chain	Res	Type
1	A	128	SER

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Mol	Chain	Res	Type
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
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	263	GLN

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Mol	Chain	Res	Type
1	A	378	GLN
1	B	195	ASN
1	B	371	GLN
1	B	378	GLN
1	B	450	ASN
1	C	246	ASN
1	C	258	GLN
1	C	284	ASN
1	C	311	ASN
1	C	342	GLN
1	C	371	GLN
1	C	378	GLN
1	D	263	GLN
1	D	311	ASN
1	D	371	GLN
1	D	378	GLN
1	D	401	ASN

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 ⓘ

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	12,14,15	0.89	1 (8%)	15,19,21	1.45	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	502	2	12,14,15	0.58	0	15,19,21	1.11	1 (6%)
2	FUC	A	503	2	9,10,11	0.90	0	10,14,16	1.01	0
2	FUL	A	504	2	9,10,11	0.84	0	10,14,16	1.42	1 (10%)
2	NAG	B	501	1,2	12,14,15	0.97	1 (8%)	15,19,21	1.06	1 (6%)
2	NAG	B	502	2	12,14,15	0.65	0	15,19,21	1.06	0
2	FUC	B	503	2	9,10,11	1.04	1 (11%)	10,14,16	1.14	1 (10%)
2	FUL	B	504	2	9,10,11	0.84	0	10,14,16	1.77	3 (30%)
2	NAG	C	501	1,2	12,14,15	0.70	0	15,19,21	1.78	3 (20%)
2	NAG	C	502	2	12,14,15	0.71	0	15,19,21	1.81	4 (26%)
2	FUC	C	503	2	9,10,11	1.01	0	10,14,16	1.53	2 (20%)
2	FUL	C	504	2	9,10,11	0.76	0	10,14,16	2.07	4 (40%)
2	NAG	D	501	1,2	12,14,15	0.71	1 (8%)	15,19,21	0.99	2 (13%)
2	NAG	D	502	2	12,14,15	0.90	1 (8%)	15,19,21	1.17	1 (6%)
2	FUC	D	503	2	9,10,11	0.80	0	10,14,16	0.79	0
2	FUL	D	504	2	9,10,11	0.98	1 (11%)	10,14,16	0.95	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
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	O5-C5	-2.93	1.40	1.45
2	D	502	NAG	O5-C5	-2.34	1.41	1.45
2	D	504	FUL	O5-C5	-2.26	1.41	1.45
2	D	501	NAG	O5-C5	-2.24	1.41	1.45
2	A	501	NAG	O5-C5	-2.08	1.41	1.45
2	B	503	FUC	O5-C5	-2.03	1.41	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	NAG	O5-C5-C6	4.72	111.94	106.98
2	C	504	FUL	C4-C3-C2	-4.38	104.63	110.50
2	C	501	NAG	C3-C2-N2	-3.97	105.71	111.76
2	C	501	NAG	O5-C5-C6	3.74	110.91	106.98
2	A	501	NAG	C3-C2-N2	-3.53	106.38	111.76
2	C	501	NAG	O3-C3-C2	-3.51	101.71	109.09
2	A	501	NAG	O3-C3-C2	-3.43	101.88	109.09
2	C	502	NAG	C3-C2-N2	-3.41	106.57	111.76
2	B	504	FUL	O2-C2-C3	3.38	117.47	110.18
2	D	502	NAG	C3-C2-N2	-3.20	106.90	111.76
2	A	504	FUL	C3-C4-C5	3.04	114.91	109.84
2	B	504	FUL	C4-C3-C2	-3.04	106.43	110.50
2	C	503	FUC	C6-C5-C4	-2.86	108.42	113.06
2	C	504	FUL	O2-C2-C3	2.59	115.77	110.18
2	B	504	FUL	C3-C4-C5	2.45	113.92	109.84
2	C	502	NAG	C3-C4-C5	2.36	114.41	110.20
2	A	502	NAG	C3-C2-N2	-2.33	108.21	111.76
2	C	502	NAG	C6-C5-C4	-2.29	107.46	113.00
2	D	501	NAG	C2-N2-C7	-2.24	119.32	123.09
2	C	504	FUL	O5-C5-C6	2.21	111.59	108.03
2	B	503	FUC	O2-C2-C3	-2.17	105.48	110.18
2	C	503	FUC	O2-C2-C3	-2.10	105.63	110.18
2	B	501	NAG	O5-C5-C6	2.07	109.16	106.98
2	C	504	FUL	O4-C4-C3	-2.05	105.75	110.35
2	D	501	NAG	C3-C2-N2	-2.05	108.64	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	12,14,15	0.61	0	15,19,21	1.32	1 (6%)
3	NAG	A	506	1	12,14,15	0.61	0	15,19,21	1.25	1 (6%)
3	NAG	B	505	1	12,14,15	0.73	1 (8%)	15,19,21	0.95	1 (6%)
3	NAG	B	506	1	12,14,15	0.58	0	15,19,21	1.14	2 (13%)
3	NAG	C	505	1	12,14,15	0.55	0	15,19,21	1.12	1 (6%)
3	NAG	D	505	1	12,14,15	0.67	0	15,19,21	1.12	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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	505	NAG	O5-C5	-2.21	1.41	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	NAG	O5-C5-C6	4.28	111.47	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	NAG	O5-C5-C6	4.12	111.31	106.98
3	C	505	NAG	O5-C5-C6	3.55	110.71	106.98
3	B	506	NAG	O5-C5-C6	3.40	110.55	106.98
3	D	505	NAG	O5-C5-C6	3.35	110.49	106.98
3	B	506	NAG	C3-C2-N2	-2.29	108.28	111.76
3	B	505	NAG	O5-C5-C6	2.25	109.34	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.20	18 (5%)	23 22	19, 30, 64, 96	0
1	B	321/373 (86%)	0.25	23 (7%)	15 14	19, 31, 67, 111	0
1	C	314/373 (84%)	0.28	25 (7%)	12 12	20, 33, 69, 101	0
1	D	314/373 (84%)	0.32	21 (6%)	17 17	21, 34, 69, 103	0
All	All	1266/1492 (84%)	0.26	87 (6%)	17 16	19, 32, 68, 111	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	138	LEU	8.5
1	A	440	ILE	7.4
1	D	413(A)	GLY	7.1
1	B	111	PRO	6.8
1	D	139	SER	6.4
1	C	114	LEU	6.2
1	C	138	LEU	5.9
1	D	114	LEU	5.8
1	A	140	ALA	5.5
1	D	440	ILE	5.5
1	C	139	SER	5.3
1	C	170(A)	THR	5.3
1	D	115	ILE	5.2
1	C	115	ILE	5.0
1	B	440	ILE	4.9
1	D	136	TYR	4.6
1	C	137	GLY	4.6
1	B	138	LEU	4.3
1	D	116	LEU	4.2
1	A	138	LEU	4.1
1	B	139	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	114	LEU	4.0
1	A	91	MET	4.0
1	C	168	THR	3.9
1	C	169	LEU	3.9
1	C	285	ASN	3.9
1	C	91	MET	3.8
1	D	169	LEU	3.8
1	A	113	ASP	3.8
1	C	113	ASP	3.7
1	B	452	PRO	3.7
1	B	113	ASP	3.7
1	B	91	MET	3.6
1	C	127	THR	3.6
1	A	115	ILE	3.6
1	B	116	LEU	3.6
1	D	168	THR	3.5
1	D	233	VAL	3.5
1	B	112	GLY	3.5
1	C	136	TYR	3.4
1	D	113	ASP	3.4
1	D	199	ARG	3.4
1	A	416	GLU	3.4
1	D	170(A)	THR	3.3
1	A	169	LEU	3.3
1	D	137	GLY	3.3
1	B	115	ILE	3.3
1	C	102	ARG	3.3
1	C	163	ILE	3.3
1	D	416	GLU	3.2
1	A	127	THR	3.2
1	B	170(A)	THR	3.2
1	D	285	ASN	3.1
1	A	170(A)	THR	3.1
1	B	199	ARG	3.1
1	A	114	LEU	3.1
1	B	247	VAL	3.0
1	A	139	SER	2.9
1	C	401	ASN	2.9
1	B	413(A)	GLY	2.8
1	C	166	ALA	2.8
1	A	137	GLY	2.6
1	A	168	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	170	SER	2.5
1	C	284	ASN	2.5
1	C	426	ILE	2.4
1	D	126	LEU	2.4
1	B	333	THR	2.4
1	B	163	ILE	2.4
1	D	284	ASN	2.4
1	B	168	THR	2.4
1	C	416	GLU	2.3
1	D	334	THR	2.3
1	B	127	THR	2.3
1	C	116	LEU	2.2
1	B	137	GLY	2.2
1	B	334	THR	2.2
1	C	161	THR	2.2
1	C	247	VAL	2.2
1	A	101	HIS	2.2
1	C	286	LEU	2.1
1	A	163	ILE	2.1
1	B	164	GLY	2.1
1	B	453	VAL	2.1
1	A	334	THR	2.1
1	A	116	LEU	2.0
1	D	163	ILE	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	502	14/15	0.15	-	41,57,69,84	0
2	NAG	D	502	14/15	0.17	-	53,60,75,88	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FUL	A	504	10/11	0.12	-	43,50,53,55	0
2	FUL	C	504	10/11	0.13	-	36,43,57,58	0
2	FUC	D	503	10/11	0.11	-	33,36,43,45	0
2	NAG	A	501	14/15	0.10	-	32,39,48,48	0
2	NAG	D	501	14/15	0.12	-	33,46,52,57	0
2	NAG	B	501	14/15	0.12	-	26,42,46,49	0
2	FUC	B	503	10/11	0.08	-	29,36,44,51	0
2	FUC	A	503	10/11	0.09	-	35,41,45,46	0
2	FUL	D	504	10/11	0.26	-	47,56,79,92	0
2	NAG	A	502	14/15	0.14	-	28,49,62,87	0
2	FUC	C	503	10/11	0.07	-	32,36,39,41	0
2	NAG	C	502	14/15	0.14	-	47,57,73,83	0
2	FUL	B	504	10/11	0.17	-	42,52,62,66	0
2	NAG	C	501	14/15	0.09	-	31,36,46,48	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	A	507	1/1	0.08	-	23,23,23,23	0
4	CA	B	507	1/1	0.07	-	22,22,22,22	0
4	CA	D	506	1/1	0.09	-	24,24,24,24	0
4	CA	C	506	1/1	0.05	-	25,25,25,25	0
3	NAG	B	505	14/15	0.31	-	76,88,100,117	0
3	NAG	C	505	14/15	0.32	-	73,84,92,102	0
3	NAG	B	506	14/15	0.36	-	72,85,96,99	0
3	NAG	D	505	14/15	0.28	-	67,81,86,90	0
3	NAG	A	506	14/15	0.22	-	71,84,95,103	0
3	NAG	A	505	14/15	0.38	-	68,86,96,97	0

6.5 Other polymers

There are no such residues in this entry.