



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:45 PM GMT

PDB ID : 1V0Z
Title : STRUCTURE OF NEURAMINIDASE FROM ENGLISH DUCK SUBTYPE N6
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on : 2004-04-02
Resolution : 1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

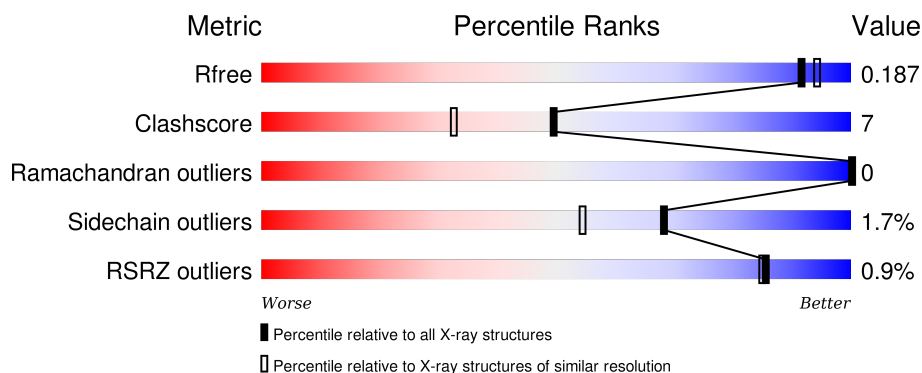
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	389	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	389	<div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	389	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
1	D	389	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEG	C	1478	-	-	X	X
2	CA	C	1477	-	-	-	X
2	CA	D	1477	-	-	-	X
3	GOL	A	1478	-	-	-	X
3	GOL	B	1478	-	-	-	X
3	GOL	C	1479	-	-	-	X
3	GOL	D	1478	-	-	-	X
4	NAG	C	1483	-	-	-	X
5	NAG	B	1482	-	-	X	X
5	NAG	D	1481	-	-	X	X
6	MAN	A	1483	-	-	-	X
6	NAG	A	1495	-	-	-	X
7	MAN	A	1485	-	-	-	X
7	MAN	A	1494	-	-	-	X
7	MAN	B	1485	-	-	-	X
7	MAN	C	1485	-	-	-	X
8	NAG	A	1488	-	-	-	X
8	MAN	A	1493	-	-	-	X
9	NAG	B	1487	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14347 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	B	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	C	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

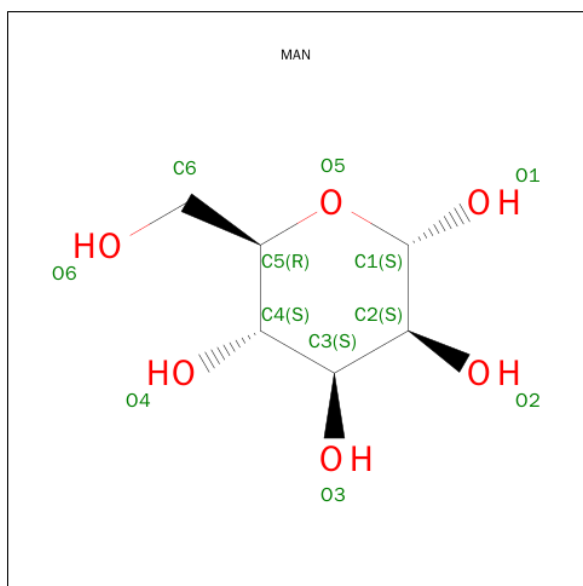


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			47	26	1	20		

- Molecule 7 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			11	6	5			
7	A	1	Total	C	O		0	0
			11	6	5			
7	A	1	Total	C	O		0	0
			11	6	5			
7	B	1	Total	C	O		0	0
			11	6	5			
7	B	1	Total	C	O		0	0
			11	6	5			
7	C	1	Total	C	O		0	0
			11	6	5			
7	D	1	Total	C	O		0	0
			11	6	5			

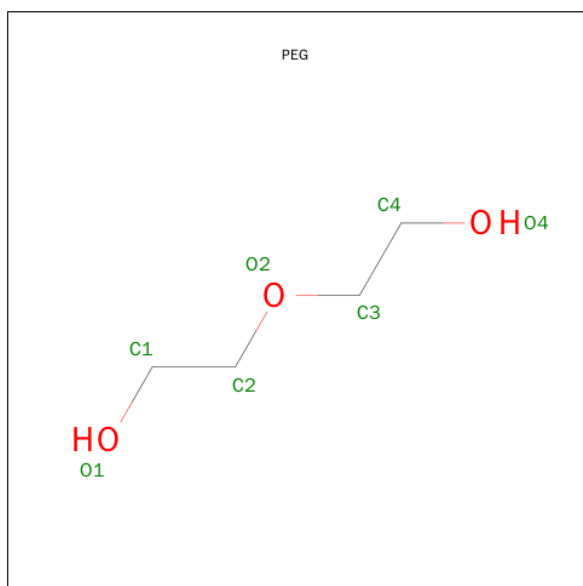
- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	2	Total	C	O	0	0
			22	12	10		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	453	Total	O	0	0
			453	453		
12	B	434	Total	O	0	0
			434	434		
12	C	450	Total	O	0	0
			450	450		

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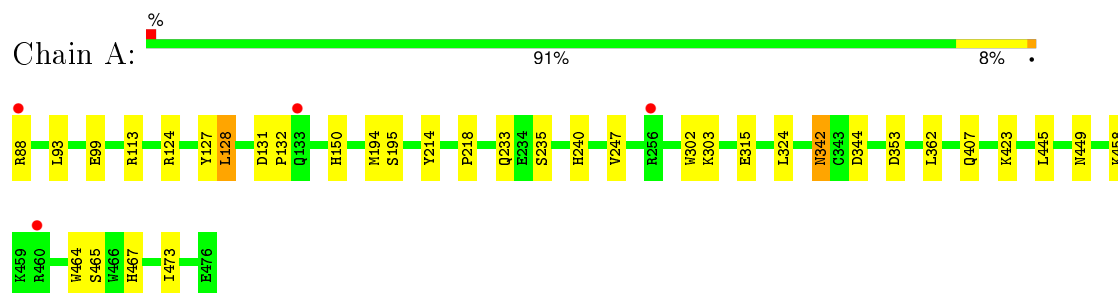
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	461	Total	O	0	0
			461	461		

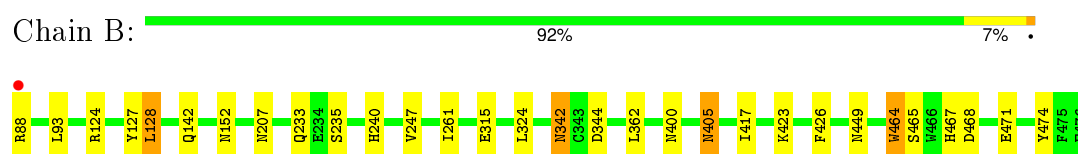
3 Residue-property plots

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.

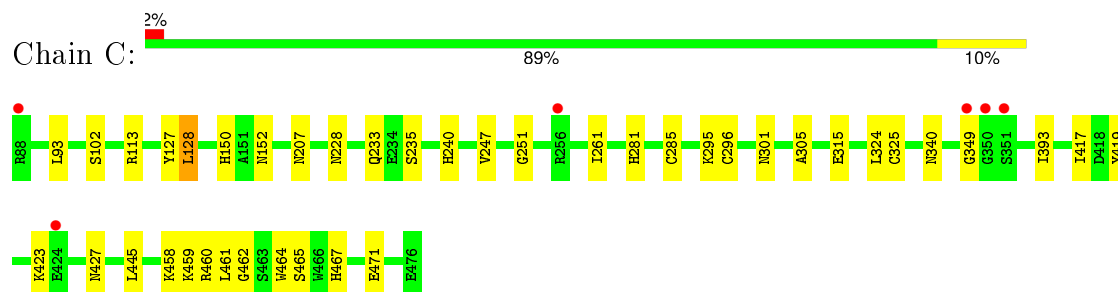
• Molecule 1: NEURAMINIDASE



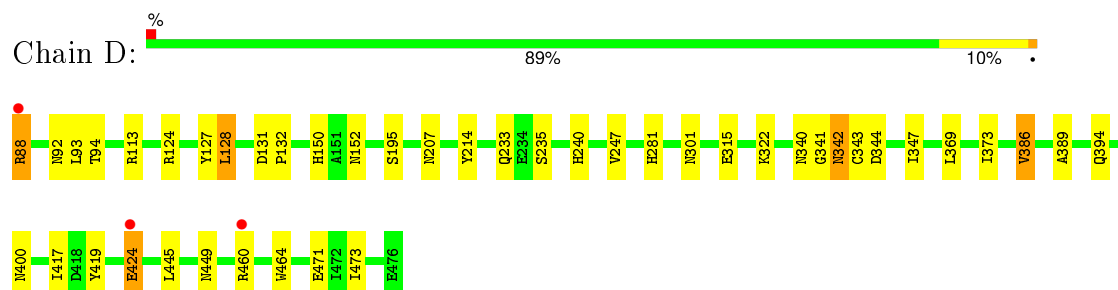
• Molecule 1: NEURAMINIDASE



• Molecule 1: NEURAMINIDASE



• Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.48Å 73.75Å 106.81Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.96 – 1.84 19.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.84) 93.2 (19.98-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.149 , 0.190 0.150 , 0.187	Depositor DCC
R_{free} test set	6696 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.4	EDS
Estimated twinning fraction	0.006 for l,k,-h 0.016 for h,-k,-l 0.012 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 133791 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14347	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, CA, PEG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/3084	0.67	1/4185 (0.0%)
1	B	0.65	1/3084 (0.0%)	0.67	1/4185 (0.0%)
1	C	0.66	0/3084	0.66	1/4185 (0.0%)
1	D	0.65	0/3084	0.69	1/4185 (0.0%)
All	All	0.65	1/12336 (0.0%)	0.67	4/16740 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	TRP	CB-CG	-5.11	1.41	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	LEU	CA-CB-CG	7.07	131.57	115.30
1	D	128	LEU	CA-CB-CG	6.70	130.71	115.30
1	B	128	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	128	LEU	CA-CB-CG	6.12	129.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3009	0	2885	26	0
1	B	3009	0	2888	30	0
1	C	3009	0	2888	51	0
1	D	3009	0	2888	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	28	0	25	0	0
4	C	28	0	25	6	0
5	A	28	0	26	0	0
5	B	56	0	52	11	0
5	C	42	0	39	5	0
5	D	42	0	39	13	0
6	A	47	0	40	4	0
7	A	33	0	30	4	0
7	B	22	0	20	0	0
7	C	11	0	10	1	0
7	D	11	0	10	2	0
8	A	72	0	61	6	0
9	B	36	0	31	5	0
10	C	7	0	10	16	0
11	C	22	0	19	5	0
12	A	453	0	0	5	0
12	B	434	0	0	1	0
12	C	450	0	0	6	0
12	D	461	0	0	1	0
All	All	14347	0	12018	163	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 7.

The worst 5 of 163 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:D:207:ASN:HD21	5:D:1481:NAG:C1	1.03	1.63
1:D:152:ASN:HD21	5:D:1480:NAG:C1	1.01	1.55
1:B:152:ASN:HD21	5:B:1480:NAG:C1	0.97	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ASN:HD21	5:C:1481:NAG:C1	0.92	1.53
1:C:207:ASN:HD21	4:C:1483:NAG:C1	0.94	1.52

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	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	B	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
1	C	387/389 (100%)	374 (97%)	13 (3%)	0	100	100
1	D	387/389 (100%)	373 (96%)	14 (4%)	0	100	100
All	All	1548/1556 (100%)	1497 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	331/331 (100%)	327 (99%)	4 (1%)	78	69
1	B	331/331 (100%)	325 (98%)	6 (2%)	66	52
1	C	331/331 (100%)	327 (99%)	4 (1%)	78	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	331/331 (100%)	323 (98%)	8 (2%)	57 39
All	All	1324/1324 (100%)	1302 (98%)	22 (2%)	68 54

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	464	TRP
1	C	445	LEU
1	D	460	ARG
1	C	128	LEU
1	C	324	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	ASN
1	C	207	ASN
1	D	406	ASN
1	B	427	ASN
1	B	467	HIS

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 ⓘ

19 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
4	NAG	A	1479	1,4	14,14,15	0.62	0	15,19,21	0.86	0
4	NAG	A	1480	4	14,14,15	0.53	0	15,19,21	0.74	1 (6%)
6	MAN	A	1483	7,6	11,11,12	0.56	0	14,15,17	1.50	2 (14%)
6	BMA	A	1486	6	11,11,12	0.26	0	14,15,17	1.29	2 (14%)
6	MAN	A	1487	6	11,11,12	0.40	0	14,15,17	0.89	0
8	NAG	A	1488	1,8	14,14,15	0.75	0	15,19,21	2.47	5 (33%)
8	NAG	A	1489	8	14,14,15	0.60	0	15,19,21	1.51	2 (13%)
8	BMA	A	1490	8	11,11,12	0.54	0	14,15,17	1.05	1 (7%)
8	MAN	A	1491	8	11,11,12	0.50	0	14,15,17	0.87	1 (7%)
8	MAN	A	1492	8	11,11,12	0.42	0	14,15,17	0.96	1 (7%)
8	MAN	A	1493	8,7	11,11,12	0.40	0	14,15,17	1.38	2 (14%)
6	NAG	A	1495	5,6	14,14,15	0.57	0	15,19,21	0.62	0
9	MAN	B	1483	9,7	11,11,12	0.43	0	14,15,17	1.08	1 (7%)
9	BMA	B	1486	9	11,11,12	0.40	0	14,15,17	1.24	1 (7%)
9	NAG	B	1487	9	14,14,15	0.65	0	15,19,21	2.50	5 (33%)
4	NAG	C	1483	1,4	14,14,15	0.59	0	15,19,21	1.67	3 (20%)
4	NAG	C	1484	4	14,14,15	0.58	0	15,19,21	0.54	0
11	BMA	C	1486	11	11,11,12	0.42	0	14,15,17	1.11	1 (7%)
11	MAN	C	1487	11	11,11,12	0.47	0	14,15,17	1.69	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1479	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1480	4	-	0/6/23/26	0/1/1/1
6	MAN	A	1483	7,6	-	0/2/19/22	0/1/1/1
6	BMA	A	1486	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1487	6	-	0/2/19/22	0/1/1/1
8	NAG	A	1488	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1489	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1490	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1491	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1492	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1493	8,7	-	0/2/19/22	0/1/1/1
6	NAG	A	1495	5,6	-	0/6/23/26	0/1/1/1
9	MAN	B	1483	9,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	B	1486	9	-	0/2/19/22	0/1/1/1
9	NAG	B	1487	9	-	0/6/23/26	0/1/1/1
4	NAG	C	1483	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1484	4	-	0/6/23/26	0/1/1/1
11	BMA	C	1486	11	-	0/2/19/22	0/1/1/1
11	MAN	C	1487	11	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1488	NAG	C3-C4-C5	-6.14	99.49	110.20
9	B	1487	NAG	C4-C3-C2	-5.33	102.94	111.23
4	C	1483	NAG	C1-O5-C5	-4.53	106.50	112.25
8	A	1488	NAG	C1-O5-C5	-3.98	107.20	112.25
11	C	1487	MAN	C2-C3-C4	-3.51	105.07	111.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1483	MAN	2	0
8	A	1488	NAG	3	0
8	A	1493	MAN	3	0
6	A	1495	NAG	2	0
9	B	1487	NAG	5	0
4	C	1483	NAG	3	0
4	C	1484	NAG	3	0
11	C	1486	BMA	3	0
11	C	1487	MAN	2	0

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	GOL	A	1478	-	5,5,5	1.17	0	5,5,5	1.81	1 (20%)
5	NAG	A	1481	1	14,14,15	0.62	0	15,19,21	0.81	0
5	NAG	A	1482	-	14,14,15	0.52	0	15,19,21	1.01	1 (6%)
7	MAN	A	1484	6	11,11,12	0.36	0	14,15,17	1.53	2 (14%)
7	MAN	A	1485	6	11,11,12	0.50	0	14,15,17	1.44	2 (14%)
7	MAN	A	1494	8	11,11,12	0.58	0	14,15,17	1.91	4 (28%)
3	GOL	B	1478	-	5,5,5	1.69	1 (20%)	5,5,5	2.13	3 (60%)
5	NAG	B	1479	-	14,14,15	0.43	0	15,19,21	1.20	2 (13%)
5	NAG	B	1480	1	14,14,15	0.68	0	15,19,21	1.09	1 (6%)
5	NAG	B	1481	-	14,14,15	0.50	0	15,19,21	1.03	1 (6%)
5	NAG	B	1482	6	14,14,15	0.55	0	15,19,21	1.40	3 (20%)
7	MAN	B	1484	9	11,11,12	0.37	0	14,15,17	1.22	2 (14%)
7	MAN	B	1485	-	11,11,12	0.50	0	14,15,17	1.95	3 (21%)
10	PEG	C	1478	-	6,6,6	0.26	0	5,5,5	5.99	4 (80%)
3	GOL	C	1479	-	5,5,5	1.59	1 (20%)	5,5,5	2.11	2 (40%)
5	NAG	C	1480	-	14,14,15	0.53	0	15,19,21	1.43	3 (20%)
5	NAG	C	1481	1	14,14,15	0.64	0	15,19,21	1.21	1 (6%)
5	NAG	C	1482	-	14,14,15	0.48	0	15,19,21	0.74	0
7	MAN	C	1485	8	11,11,12	0.42	0	14,15,17	1.66	2 (14%)
3	GOL	D	1478	-	5,5,5	1.35	0	5,5,5	1.87	1 (20%)
5	NAG	D	1479	-	14,14,15	0.44	0	15,19,21	1.04	0
5	NAG	D	1480	1	14,14,15	0.58	0	15,19,21	1.30	1 (6%)
5	NAG	D	1481	1	14,14,15	0.60	0	15,19,21	1.81	3 (20%)
7	MAN	D	1483	-	11,11,12	0.58	0	14,15,17	1.30	2 (14%)

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	GOL	A	1478	-	-	0/4/4/4	0/0/0/0
5	NAG	A	1481	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1482	-	-	0/6/23/26	0/1/1/1
7	MAN	A	1484	6	-	0/2/19/22	0/1/1/1
7	MAN	A	1485	6	-	0/2/19/22	0/1/1/1
7	MAN	A	1494	8	-	0/2/19/22	0/1/1/1
3	GOL	B	1478	-	-	0/4/4/4	0/0/0/0
5	NAG	B	1479	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1480	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1481	-	-	0/6/23/26	0/1/1/1
5	NAG	B	1482	6	-	0/6/23/26	0/1/1/1
7	MAN	B	1484	9	-	0/2/19/22	0/1/1/1
7	MAN	B	1485	-	-	0/2/19/22	0/1/1/1
10	PEG	C	1478	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1479	-	-	0/4/4/4	0/0/0/0
5	NAG	C	1480	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1481	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1482	-	-	0/6/23/26	0/1/1/1
7	MAN	C	1485	8	-	0/2/19/22	0/1/1/1
3	GOL	D	1478	-	-	0/4/4/4	0/0/0/0
5	NAG	D	1479	-	-	0/6/23/26	0/1/1/1
5	NAG	D	1480	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1481	1	-	0/6/23/26	0/1/1/1
7	MAN	D	1483	-	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1479	GOL	O3-C3	2.29	1.52	1.42
3	B	1478	GOL	O3-C3	2.65	1.53	1.42

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1478	PEG	C3-O2-C2	-6.20	86.66	113.31
5	D	1481	NAG	C1-O5-C5	-4.67	106.32	112.25
5	D	1480	NAG	C1-O5-C5	-3.80	107.42	112.25
5	C	1481	NAG	C1-O5-C5	-2.73	108.78	112.25
7	A	1494	MAN	O2-C2-C1	-2.61	103.98	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1478	GOL	2	0
7	A	1484	MAN	1	0
7	A	1485	MAN	1	0
7	A	1494	MAN	2	0
3	B	1478	GOL	1	0
5	B	1480	NAG	3	0
5	B	1482	NAG	8	0
10	C	1478	PEG	16	0
3	C	1479	GOL	1	0
5	C	1481	NAG	4	0
5	C	1482	NAG	1	0
7	C	1485	MAN	1	0
5	D	1479	NAG	3	0
5	D	1480	NAG	3	0
5	D	1481	NAG	7	0
7	D	1483	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	389/389 (100%)	-0.45	4 (1%) 84 83	7, 12, 20, 31	0
1	B	389/389 (100%)	-0.47	1 (0%) 94 93	7, 12, 18, 37	0
1	C	389/389 (100%)	-0.49	6 (1%) 76 74	7, 11, 19, 33	0
1	D	389/389 (100%)	-0.45	3 (0%) 87 86	7, 12, 18, 33	0
All	All	1556/1556 (100%)	-0.46	14 (0%) 85 85	7, 12, 19, 37	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	4.3
1	C	350	GLY	3.6
1	C	349	GLY	3.3
1	A	88	ARG	3.2
1	C	88	ARG	2.9

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(\AA^2)	Q<0.9
4	NAG	C	1483	14/15	0.86	0.24	12.69	25,29,32,34	0
9	NAG	B	1487	14/15	0.69	0.26	11.35	26,35,39,43	0
6	MAN	A	1483	11/12	0.90	0.20	7.38	22,24,24,27	0
8	MAN	A	1493	11/12	0.95	0.14	5.41	14,15,16,19	0
8	NAG	A	1488	14/15	0.81	0.32	4.24	26,31,35,38	0
6	NAG	A	1495	14/15	0.80	0.28	2.32	20,24,27,30	0
4	NAG	C	1484	14/15	0.81	0.21	1.59	18,24,29,33	0
8	NAG	A	1489	14/15	0.92	0.15	1.00	14,20,24,25	0
9	BMA	B	1486	11/12	0.85	0.24	-	35,36,37,38	0
6	BMA	A	1486	11/12	0.94	0.21	-	21,25,26,31	0
4	NAG	A	1480	14/15	0.68	0.45	-	39,43,45,45	0
8	MAN	A	1492	11/12	0.84	0.41	-	38,42,44,44	0
11	MAN	C	1487	11/12	0.60	0.42	-	45,49,51,51	0
8	MAN	A	1491	11/12	0.94	0.13	-	24,25,27,27	0
4	NAG	A	1479	14/15	0.90	0.16	-	20,22,26,32	0
8	BMA	A	1490	11/12	0.94	0.13	-	16,19,19,21	0
9	MAN	B	1483	11/12	0.82	0.26	-	35,37,37,37	0
11	BMA	C	1486	11/12	0.85	0.28	-	32,35,36,40	0
6	MAN	A	1487	11/12	0.76	0.44	-	45,48,49,50	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
7	MAN	B	1485	11/12	0.74	0.33	12.17	44,47,48,49	0
3	GOL	B	1478	6/6	0.67	0.28	9.34	12,25,26,28	0
3	GOL	D	1478	6/6	0.73	0.29	7.34	17,29,30,30	0
3	GOL	C	1479	6/6	0.76	0.26	7.12	13,26,28,29	0
7	MAN	A	1485	11/12	0.85	0.18	6.45	24,27,28,29	0
5	NAG	D	1481	14/15	0.82	0.21	6.34	23,26,27,27	0
3	GOL	A	1478	6/6	0.69	0.24	6.32	19,29,30,31	0
10	PEG	C	1478	7/7	0.67	0.25	6.31	20,24,28,29	0
2	CA	C	1477	1/1	0.98	0.17	5.29	19,19,19,19	0
2	CA	D	1477	1/1	0.99	0.13	3.76	19,19,19,19	0
7	MAN	A	1494	11/12	0.92	0.14	3.57	19,20,21,21	0
7	MAN	C	1485	11/12	0.85	0.19	2.99	30,33,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	1482	14/15	0.73	0.30	2.01	42,44,45,45	0
2	CA	B	1477	1/1	0.99	0.09	1.68	19,19,19,19	0
2	CA	A	1477	1/1	0.99	0.14	1.36	20,20,20,20	0
5	NAG	B	1481	14/15	0.15	0.47	-	95,96,97,97	0
5	NAG	C	1482	14/15	0.42	0.37	-	74,77,77,77	0
5	NAG	A	1482	14/15	0.47	0.49	-	64,67,68,68	0
5	NAG	B	1480	14/15	0.90	0.14	-	16,22,26,29	0
5	NAG	A	1481	14/15	0.89	0.16	-	19,22,27,28	0
5	NAG	C	1481	14/15	0.93	0.13	-	15,18,25,26	0
7	MAN	D	1483	11/12	0.53	0.39	-	67,68,68,68	0
7	MAN	A	1484	11/12	0.81	0.20	-	26,30,35,38	0
5	NAG	C	1480	14/15	0.47	0.37	-	62,63,64,64	0
5	NAG	D	1480	14/15	0.92	0.15	-	17,22,26,26	0
5	NAG	B	1479	14/15	0.31	0.43	-	98,99,99,99	0
7	MAN	B	1484	11/12	0.79	0.29	-	32,33,36,38	0
5	NAG	D	1479	14/15	0.50	0.43	-	105,105,106,106	0

6.5 Other polymers

There are no such residues in this entry.