



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 22, 2016 – 07:33 PM EST

PDB ID : 1U8E
Title : HUMAN DIPEPTIDYL PEPTIDASE IV/CD26 MUTANT Y547F
Authors : Bjelke, J.R.; Christensen, J.; Branner, S.; Wagtmann, N.; Olsen, C.; Kanstrup, A.B.; Rasmussen, H.B.
Deposited on : 2004-08-05
Resolution : 2.20 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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) : rb-20028320

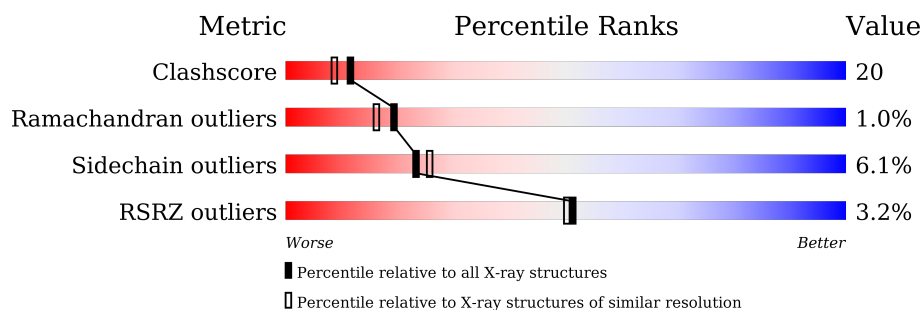
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	728	<div> <div>2%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
1	B	728	<div> <div>4%</div> <div>63%</div> <div>32%</div> <div>5%</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	NDG	B	779	-	-	-	X
2	NAG	B	767	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	774	-	-	-	X
4	NDG	B	771	-	-	-	X
4	NAG	B	772	-	-	-	X
6	NAG	A	780	-	-	-	X
7	NAG	A	782	-	-	-	X
7	NAG	B	781	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13182 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 Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5946	3816	980	1124	26			
1	B	728	Total	C	N	O	S	0	0	0
			5961	3827	982	1126	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	PHE	TYR	ENGINEERED	UNP P27487
B	547	PHE	TYR	ENGINEERED	UNP P27487

- 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
			38	22	2	14		
2	B	3	Total	C	N	O	0	0
			38	22	2	14		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		

- 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	B	2	Total	C	N	O	0	0
			28	16	2	10		

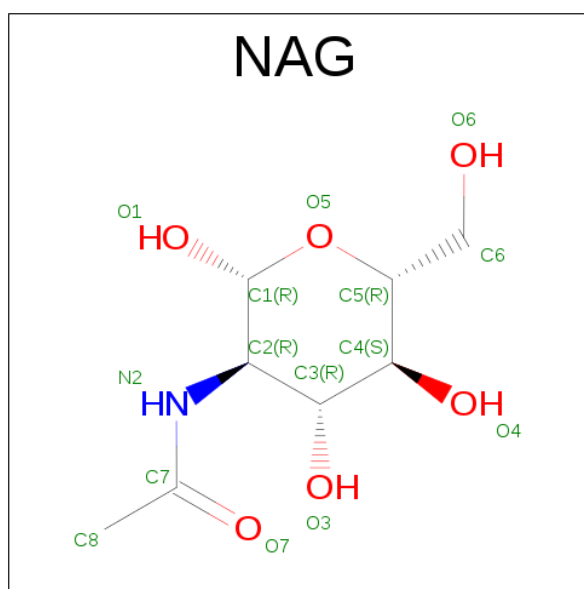
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	3	Total	C	N	O	0	0
			39	22	2	15		

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

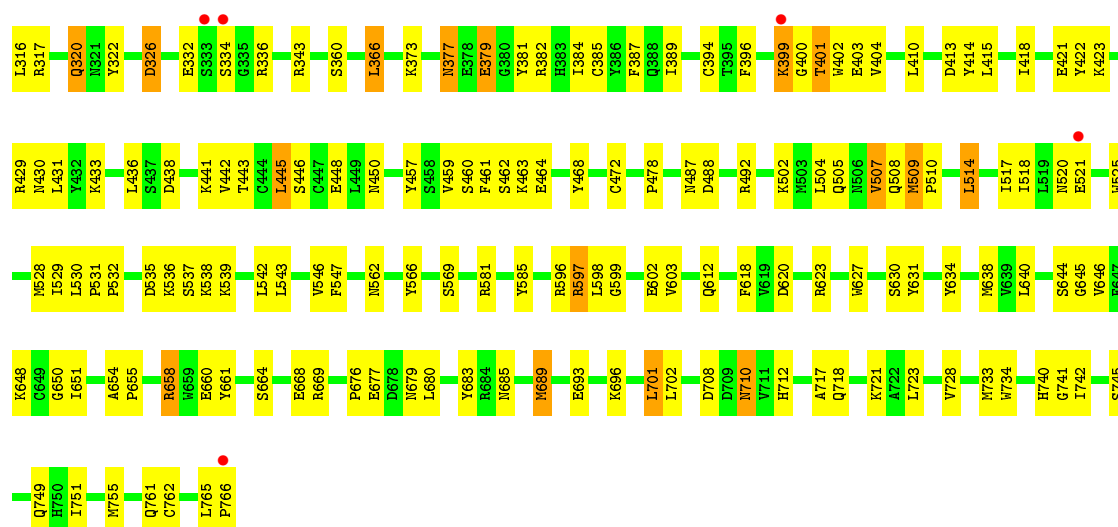
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	448	Total	O	0	0
			448	448		
11	B	414	Total	O	0	0
			414	414		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.76Å 121.37Å 129.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.84 – 2.20 38.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.5 (34.84-2.20) 70.0 (38.61-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.10Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.215 , 0.268 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13182	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MAN, BMA, NAG, NDG, 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	0.32	0/6117	0.63	0/8318
1	B	0.32	0/6133	0.63	1/8341 (0.0%)
All	All	0.32	0/12250	0.63	1/16659 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	LEU	N-CA-C	-5.02	97.43	111.00

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	5946	0	5656	225	0
1	B	5961	0	5673	252	0
2	A	38	0	34	4	0
2	B	38	0	34	3	0
3	A	38	0	34	5	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
5	A	39	0	34	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	56	0	50	3	0
7	A	14	0	13	5	0
7	B	28	0	26	10	0
8	B	39	0	34	0	0
9	B	39	0	34	1	0
10	B	28	0	25	1	0
11	A	448	0	0	23	0
11	B	414	0	0	28	0
All	All	13182	0	11697	491	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 20.

The worst 5 of 491 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:492:ARG:HH11	1:A:492:ARG:HB3	1.25	0.97
1:B:258:LYS:HZ1	1:B:712:HIS:CD2	1.86	0.93
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.48	0.93
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.49	0.92
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	0.96	0.90

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	724/728 (100%)	664 (92%)	53 (7%)	7 (1%)	19	16
1	B	726/728 (100%)	669 (92%)	49 (7%)	8 (1%)	17	14
All	All	1450/1456 (100%)	1333 (92%)	102 (7%)	15 (1%)	19	16

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	A	320	GLN
1	A	520	ASN
1	B	399	LYS
1	B	401	THR

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	650/653 (100%)	615 (95%)	35 (5%)	27	31
1	B	652/653 (100%)	608 (93%)	44 (7%)	20	21
All	All	1302/1306 (100%)	1223 (94%)	79 (6%)	23	26

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	41	LYS
1	B	139	LYS
1	B	685	ASN
1	B	57	LEU
1	B	73	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	B	112	GLN
1	B	710	ASN
1	B	51	ASN
1	B	72	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 ⓘ

28 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	767	1,2	14,14,15	0.65	0	15,19,21	1.19	1 (6%)
2	NAG	A	768	2	14,14,15	0.43	0	15,19,21	0.80	1 (6%)
2	FUC	A	769	2	10,10,11	0.58	0	13,14,16	0.69	0
3	NDG	A	770	1,3	14,14,15	1.00	1 (7%)	15,19,21	0.78	0
3	NAG	A	771	3	14,14,15	0.79	1 (7%)	15,19,21	0.61	0
3	FUC	A	772	3	10,10,11	0.57	0	13,14,16	0.39	0
4	NDG	A	773	1,4	14,14,15	0.93	0	15,19,21	1.29	2 (13%)
4	NAG	A	774	4	14,14,15	0.57	0	15,19,21	0.85	1 (6%)
5	NAG	A	775	1,5	14,14,15	0.72	0	15,19,21	0.89	1 (6%)
5	NDG	A	776	5	14,14,15	0.85	0	15,19,21	1.49	3 (20%)
5	MAN	A	777	5	11,11,12	0.79	0	15,15,17	0.56	0
6	NAG	A	778	1,6	14,14,15	0.61	0	15,19,21	0.83	1 (6%)
6	NAG	A	779	6	14,14,15	0.51	0	15,19,21	0.76	0
6	NAG	A	780	1,6	14,14,15	0.60	0	15,19,21	0.75	1 (6%)
6	NAG	A	781	6	14,14,15	0.61	0	15,19,21	0.86	0
2	NAG	B	767	1,2	14,14,15	0.62	0	15,19,21	1.01	0
2	NAG	B	768	2	14,14,15	0.57	0	15,19,21	1.07	1 (6%)
2	FUC	B	769	2	10,10,11	0.57	0	13,14,16	0.61	0
4	NDG	B	771	1,4	14,14,15	0.71	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	772	4	14,14,15	0.66	0	15,19,21	0.91	1 (6%)
8	NDG	B	773	1,8	14,14,15	0.98	1 (7%)	15,19,21	1.25	2 (13%)
8	NAG	B	774	8	14,14,15	0.73	0	15,19,21	0.85	1 (6%)
8	BMA	B	775	8	11,11,12	0.46	0	15,15,17	0.47	0
9	NAG	B	776	1,9	14,14,15	1.05	1 (7%)	15,19,21	1.30	2 (13%)
9	NDG	B	777	9	14,14,15	0.95	0	15,19,21	0.93	1 (6%)
9	BMA	B	778	9	11,11,12	0.62	0	15,15,17	0.63	0
10	NDG	B	779	1,10	14,14,15	0.68	0	15,19,21	0.94	1 (6%)
10	NDG	B	780	10	14,14,15	0.54	0	15,19,21	1.11	2 (13%)

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	767	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	768	2	-	0/6/23/26	0/1/1/1
2	FUC	A	769	2	-	0/0/17/20	0/1/1/1
3	NDG	A	770	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	771	3	-	0/6/23/26	0/1/1/1
3	FUC	A	772	3	-	0/0/17/20	0/1/1/1
4	NDG	A	773	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	774	4	-	0/6/23/26	0/1/1/1
5	NAG	A	775	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	776	5	-	0/6/23/26	0/1/1/1
5	MAN	A	777	5	-	0/2/19/22	0/1/1/1
6	NAG	A	778	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	779	6	-	0/6/23/26	0/1/1/1
6	NAG	A	780	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	781	6	-	0/6/23/26	0/1/1/1
2	NAG	B	767	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	768	2	-	0/6/23/26	0/1/1/1
2	FUC	B	769	2	-	0/0/17/20	0/1/1/1
4	NDG	B	771	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	772	4	-	0/6/23/26	0/1/1/1
8	NDG	B	773	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	774	8	-	0/6/23/26	0/1/1/1
8	BMA	B	775	8	-	0/2/19/22	0/1/1/1
9	NAG	B	776	1,9	-	0/6/23/26	0/1/1/1
9	NDG	B	777	9	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	B	778	9	-	0/2/19/22	0/1/1/1
10	NDG	B	779	1,10	-	0/6/23/26	0/1/1/1
10	NDG	B	780	10	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	773	NDG	C1-C2	2.33	1.55	1.52
3	A	771	NAG	C1-C2	2.34	1.55	1.52
3	A	770	NDG	C1-C2	2.44	1.55	1.52
9	B	776	NAG	C1-C2	2.61	1.56	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	776	NDG	C2-N2-C7	-3.81	118.15	123.11
9	B	776	NAG	C2-N2-C7	-3.35	118.75	123.11
2	B	768	NAG	C2-N2-C7	-3.14	119.02	123.11
5	A	775	NAG	C2-N2-C7	-2.96	119.25	123.11
10	B	779	NDG	C2-N2-C7	-2.92	119.31	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	NAG	2	0
2	A	768	NAG	4	0
2	A	769	FUC	2	0
3	A	770	NDG	4	0
3	A	771	NAG	4	0
5	A	775	NAG	3	0
5	A	776	NDG	4	0
5	A	777	MAN	2	0
6	A	779	NAG	2	0
6	A	780	NAG	1	0
2	B	767	NAG	2	0
2	B	768	NAG	1	0
2	B	769	FUC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	771	NDG	1	0
9	B	777	NDG	1	0
10	B	779	NDG	1	0
10	B	780	NDG	1	0

5.6 Ligand geometry

3 ligands 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$
7	NAG	A	782	1	14,14,15	0.73	1 (7%)	15,19,21	0.69	0
7	NAG	B	770	1	14,14,15	0.58	0	15,19,21	0.85	1 (6%)
7	NAG	B	781	1	14,14,15	0.90	1 (7%)	15,19,21	0.80	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
7	NAG	A	782	1	-	0/6/23/26	0/1/1/1
7	NAG	B	770	1	-	0/6/23/26	0/1/1/1
7	NAG	B	781	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	782	NAG	C1-C2	2.20	1.55	1.52
7	B	781	NAG	C1-C2	2.59	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	B	770	NAG	C2-N2-C7	-2.46	119.91	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	782	NAG	5	0
7	B	770	NAG	2	0
7	B	781	NAG	8	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	726/728 (99%)	-0.23	17 (2%) 64 63	9, 24, 49, 68	0
1	B	728/728 (100%)	-0.15	29 (3%) 42 41	9, 24, 53, 74	0
All	All	1454/1456 (99%)	-0.19	46 (3%) 51 50	9, 24, 51, 74	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	GLU	6.8
1	B	39	SER	5.6
1	B	92	ASN	5.5
1	B	97	GLU	5.1
1	A	279	VAL	4.8

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
4	NDG	B	771	14/15	0.71	0.27	5.94	54,59,62,63	0
10	NDG	B	779	14/15	0.59	0.25	5.81	56,60,63,69	0
6	NAG	A	780	14/15	0.83	0.18	4.86	47,51,55,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	774	14/15	0.69	0.27	3.88	63,66,66,67	0
4	NAG	B	772	14/15	0.62	0.30	3.68	66,68,68,68	0
2	NAG	B	767	14/15	0.80	0.28	2.27	67,69,76,76	0
2	NAG	A	767	14/15	0.76	0.21	1.60	63,66,74,74	0
9	NAG	B	776	14/15	0.84	0.12	0.89	37,41,48,56	0
5	NAG	A	775	14/15	0.88	0.10	-0.41	43,45,49,56	0
8	NDG	B	773	14/15	0.91	0.11	-0.62	30,39,45,51	0
5	NDG	A	776	14/15	0.67	0.30	-	62,65,67,70	0
9	BMA	B	778	11/12	0.28	0.48	-	80,82,83,84	0
2	FUC	B	769	10/11	0.66	0.54	-	77,79,79,79	0
3	NDG	A	770	14/15	0.54	0.40	-	71,76,78,78	0
3	NAG	A	771	14/15	0.45	0.50	-	80,81,83,84	0
3	FUC	A	772	10/11	0.70	0.49	-	78,79,79,79	0
2	NAG	B	768	14/15	0.59	0.51	-	80,83,84,85	0
8	NAG	B	774	14/15	0.77	0.24	-	58,61,66,70	0
2	NAG	A	768	14/15	0.38	0.48	-	78,79,81,81	0
9	NDG	B	777	14/15	0.54	0.32	-	64,68,72,76	0
4	NDG	A	773	14/15	0.80	0.20	-	47,51,54,59	0
5	MAN	A	777	11/12	0.47	0.49	-	72,73,74,74	0
10	NDG	B	780	14/15	0.69	0.41	-	73,76,79,79	0
6	NAG	A	778	14/15	0.72	0.27	-	63,66,67,70	0
2	FUC	A	769	10/11	0.56	0.39	-	77,78,78,78	0
8	BMA	B	775	11/12	0.60	0.28	-	73,75,77,77	0
6	NAG	A	779	14/15	0.61	0.48	-	73,76,77,77	0
6	NAG	A	781	14/15	0.57	0.32	-	63,65,66,66	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	B	781	14/15	0.62	0.49	6.76	66,68,69,69	0
7	NAG	A	782	14/15	0.48	0.48	3.86	73,76,77,77	0
7	NAG	B	770	14/15	0.67	0.33	-	60,64,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.