



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:00 PM GMT

PDB ID : 1N1M
Title : Human Dipeptidyl Peptidase IV/CD26 in complex with an inhibitor
Authors : Rasmussen, H.B.; Branner, S.; Wiberg, F.C.; Wagtmann, N.R.
Deposited on : 2002-10-18
Resolution : 2.50 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

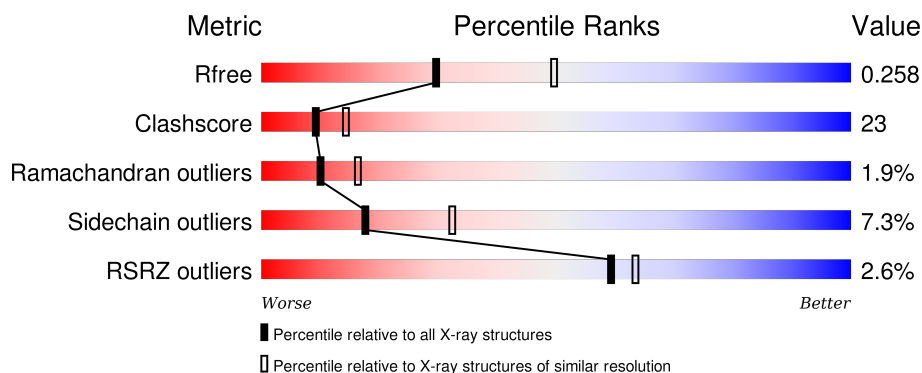
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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>63%</div> <div>32%</div> <div>5%</div> </div>
1	B	728	<div> <div>4%</div> <div>59%</div> <div>35%</div> <div>6%</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	778	-	-	-	X
2	NAG	A	767	-	-	-	X
4	NAG	A	774	-	-	-	X
5	NDG	A	776	-	-	X	-
6	NAG	A	782	-	-	X	-
6	NAG	B	780	-	-	-	X
8	NAG	B	771	-	-	-	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 13270 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 SOLUBLE FORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5964	3827	982	1129	26			

- Molecule 2 is a polymer of unknown type called NAG-NAG-FUC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	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 NAG-NAG.

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

- Molecule 5 is a polymer of unknown type called NAG-NAG-MAN.

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is a polymer of unknown type called NAG-FUC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- 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		

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

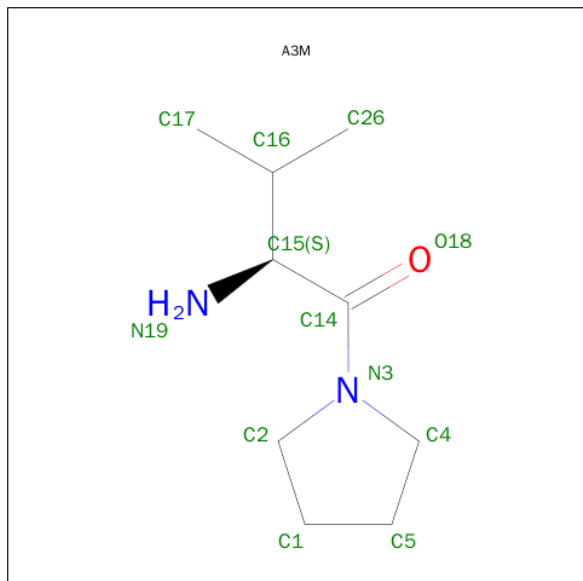
- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 11 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	2	Total	Hg	0	0
			2	2		
11	A	2	Total	Hg	0	0
			2	2		

- Molecule 12 is 2-AMINO-3-METHYL-1-PYRROLIDIN-1-YL-BUTAN-1-ONE (three-letter code: A3M) (formula: C₉H₁₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			12	9	2	1		
12	B	1	Total	C	N	O	0	0
			12	9	2	1		

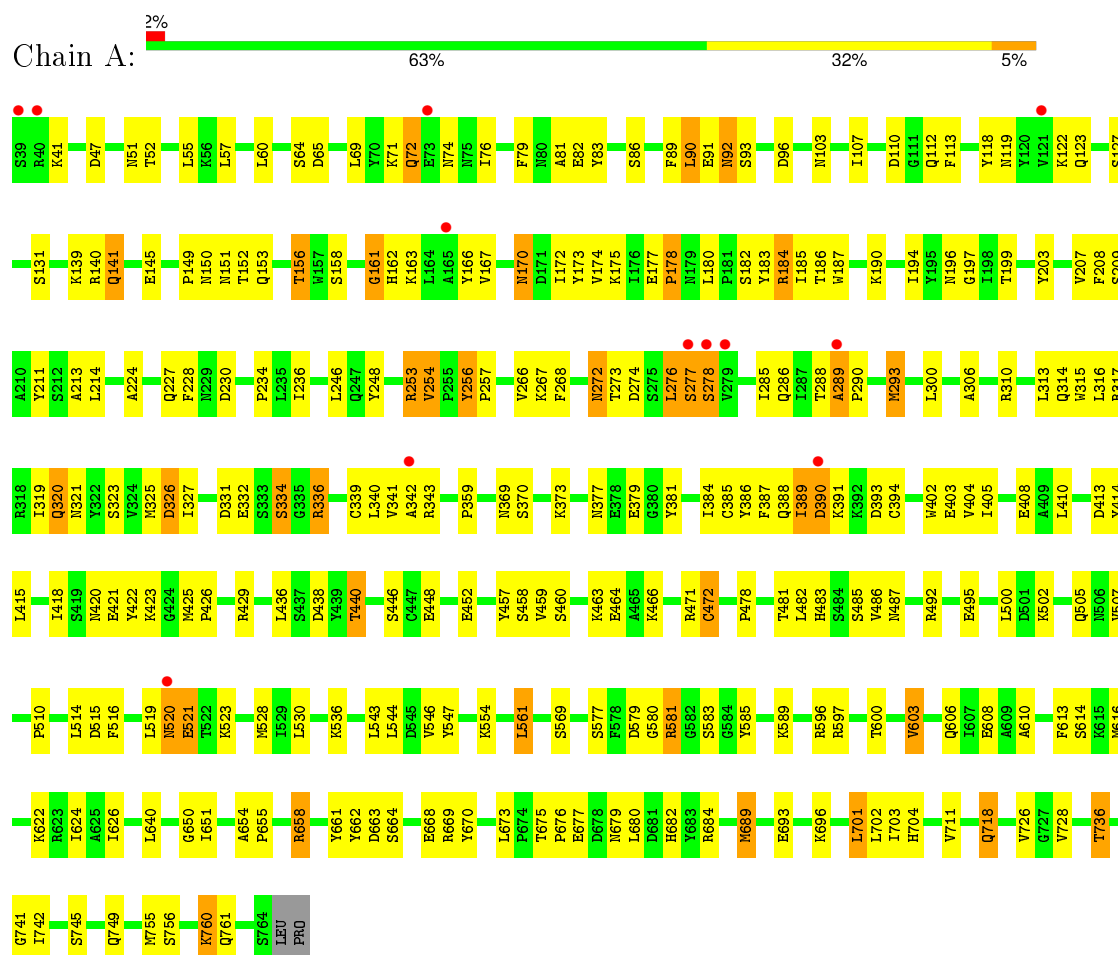
- Molecule 13 is water.

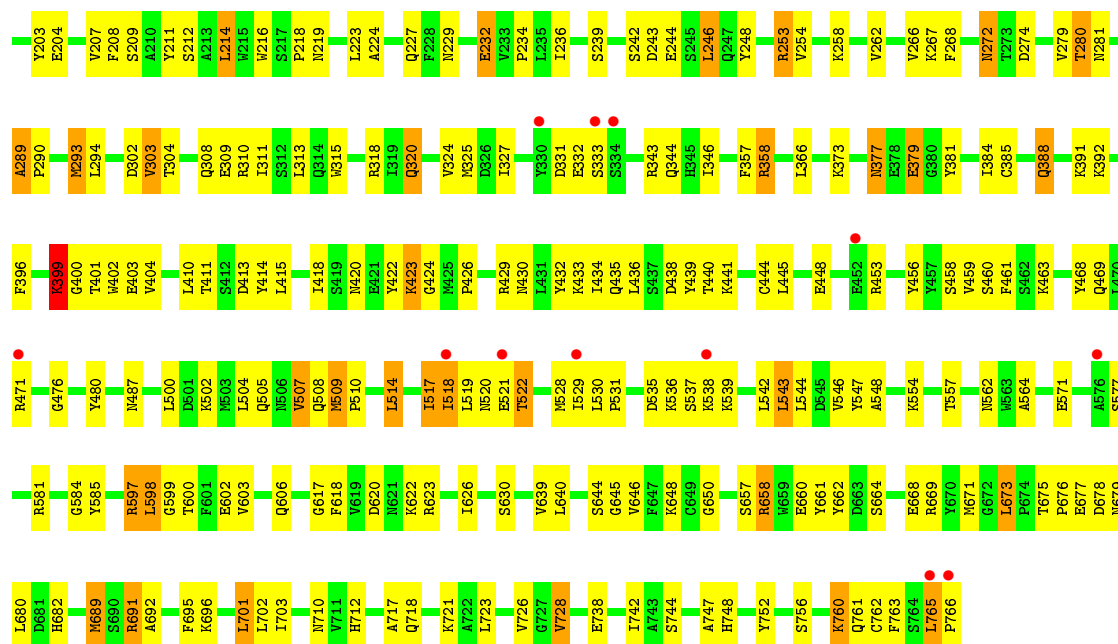
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	488	Total 488	O 488	0	0
13	B	443	Total 443	O 443	0	0

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: Dipeptidyl peptidase IV SOLUBLE FORM





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.23Å 123.45Å 131.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.50 29.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.98-2.50) 87.3 (29.98-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.51Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.208 , 0.263 0.205 , 0.258	Depositor DCC
R_{free} test set	2987 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.7	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59045 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: BMA, NAG, NDG, FUC, HG, A3M, 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	0.35	0/6119	0.65	0/8321
1	B	0.34	0/6136	0.65	1/8344 (0.0%)
All	All	0.35	0/12255	0.65	1/16665 (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	399	LYS	N-CA-C	5.19	125.02	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	5948	0	5657	247	0
1	B	5964	0	5673	282	0
2	A	38	0	34	3	0
3	A	38	0	34	8	0
4	A	84	0	75	3	0
5	A	39	0	34	11	0
6	A	14	0	13	8	0
6	B	28	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	24	0	22	2	0
8	B	28	0	25	4	0
9	B	78	0	68	1	0
10	B	28	0	25	5	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
12	A	12	0	18	2	0
12	B	12	0	18	3	0
13	A	488	0	0	15	0
13	B	443	0	0	29	0
All	All	13270	0	11722	552	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 23.

The worst 5 of 552 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)
5:A:776:NDG:H6C2	5:A:777:MAN:H2	1.26	1.13
1:A:581:ARG:CZ	6:A:782:NAG:H61	1.81	1.08
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.33	1.06
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.40	1.02
1:B:172:ILE:HG22	1:B:185:ILE:HD11	1.42	1.00

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%)	661 (91%)	50 (7%)	13 (2%)	11	18
1	B	726/728 (100%)	654 (90%)	58 (8%)	14 (2%)	10	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1450/1456 (100%)	1315 (91%)	108 (7%)	27 (2%)	10	16

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	B	289	ALA
1	B	399	LYS
1	B	645	GLY
1	B	765	LEU

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	651/653 (100%)	605 (93%)	46 (7%)	18	34
1	B	653/653 (100%)	604 (92%)	49 (8%)	17	31
All	All	1304/1306 (100%)	1209 (93%)	95 (7%)	17	32

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	B	145	GLU
1	B	689	MET
1	A	760	LYS
1	B	66	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	704	HIS
1	B	112	GLN
1	B	712	HIS

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Mol	Chain	Res	Type
1	A	718	GLN
1	B	51	ASN

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 ⓘ

27 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	0.76	0	15,19,21	1.07	1 (6%)
2	NDG	A	768	2	14,14,15	0.87	1 (7%)	15,19,21	1.22	2 (13%)
2	FUC	A	769	2	10,10,11	0.49	0	14,14,16	0.56	0
3	NDG	A	770	1,3	14,14,15	0.76	0	15,19,21	0.79	1 (6%)
3	NAG	A	771	3	14,14,15	0.84	1 (7%)	15,19,21	0.62	0
3	FUC	A	772	3	10,10,11	0.59	0	14,14,16	0.60	0
4	NAG	A	773	1,4	14,14,15	0.49	0	15,19,21	0.91	1 (6%)
4	NAG	A	774	4	14,14,15	0.54	0	15,19,21	0.56	0
5	NAG	A	775	1,5	14,14,15	0.58	0	15,19,21	0.93	1 (6%)
5	NDG	A	776	5	14,14,15	0.83	1 (7%)	15,19,21	1.21	2 (13%)
5	MAN	A	777	5	11,11,12	0.70	0	14,15,17	0.56	0
4	NAG	A	778	1,4	14,14,15	0.58	0	15,19,21	1.02	2 (13%)
4	NAG	A	779	4	14,14,15	0.60	0	15,19,21	0.61	0
4	NAG	A	780	1,4	14,14,15	0.59	0	15,19,21	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	781	4	14,14,15	0.65	0	15,19,21	0.66	0
7	NAG	B	767	1,7	14,14,15	0.61	0	15,19,21	0.81	1 (6%)
7	FUC	B	768	7	10,10,11	0.54	0	14,14,16	0.60	0
8	NDG	B	770	1,8	14,14,15	0.74	0	15,19,21	1.10	2 (13%)
8	NAG	B	771	8	14,14,15	0.55	0	15,19,21	0.61	0
9	NAG	B	772	1,9	14,14,15	0.45	0	15,19,21	0.83	1 (6%)
9	NAG	B	773	9	14,14,15	0.54	0	15,19,21	0.88	1 (6%)
9	BMA	B	774	9	11,11,12	0.64	0	14,15,17	0.37	0
9	NAG	B	775	1,9	14,14,15	0.62	0	15,19,21	0.87	1 (6%)
9	NAG	B	776	9	14,14,15	0.85	0	15,19,21	1.42	2 (13%)
9	BMA	B	777	9	11,11,12	0.73	0	14,15,17	1.11	1 (7%)
10	NDG	B	778	1,10	14,14,15	0.75	0	15,19,21	1.05	2 (13%)
10	NDG	B	779	10	14,14,15	0.76	1 (7%)	15,19,21	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	767	1,2	-	0/6/23/26	0/1/1/1
2	NDG	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	NAG	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
4	NAG	A	778	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	779	4	-	0/6/23/26	0/1/1/1
4	NAG	A	780	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	781	4	-	0/6/23/26	0/1/1/1
7	NAG	B	767	1,7	-	0/6/23/26	0/1/1/1
7	FUC	B	768	7	-	0/0/17/20	0/1/1/1
8	NDG	B	770	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	771	8	-	0/6/23/26	0/1/1/1
9	NAG	B	772	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	773	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	B	774	9	-	0/2/19/22	0/1/1/1
9	NAG	B	775	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	776	9	-	0/6/23/26	0/1/1/1
9	BMA	B	777	9	-	0/2/19/22	0/1/1/1
10	NDG	B	778	1,10	-	0/6/23/26	0/1/1/1
10	NDG	B	779	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)
10	B	779	NDG	C1-C2	2.12	1.55	1.52
5	A	776	NDG	C1-C2	2.22	1.55	1.52
2	A	768	NDG	C1-C2	2.34	1.55	1.52
3	A	771	NAG	C1-C2	2.63	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	776	NAG	C4-C3-C2	-3.51	105.78	111.23
10	B	778	NDG	C2-N2-C7	-2.82	119.42	123.04
5	A	775	NAG	C2-N2-C7	-2.77	119.48	123.04
9	B	775	NAG	C2-N2-C7	-2.64	119.65	123.04
9	B	773	NAG	C2-N2-C7	-2.62	119.68	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	NAG	2	0
2	A	768	NDG	2	0
2	A	769	FUC	1	0
3	A	770	NDG	6	0
3	A	771	NAG	6	0
3	A	772	FUC	1	0
5	A	775	NAG	6	0
5	A	776	NDG	9	0
5	A	777	MAN	3	0
4	A	779	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	780	NAG	1	0
4	A	781	NAG	2	0
7	B	767	NAG	1	0
7	B	768	FUC	1	0
8	B	770	NDG	3	0
8	B	771	NAG	1	0
9	B	777	BMA	1	0
10	B	778	NDG	5	0
10	B	779	NDG	5	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
6	NAG	A	782	1	14,14,15	0.89	1 (7%)	15,19,21	0.81	0
12	A3M	A	954	-	10,12,12	4.11	4 (40%)	13,16,16	2.57	8 (61%)
6	NAG	B	769	1	14,14,15	0.63	0	15,19,21	0.85	1 (6%)
6	NAG	B	780	1	14,14,15	0.82	0	15,19,21	0.75	1 (6%)
12	A3M	B	955	-	10,12,12	4.29	4 (40%)	13,16,16	2.50	8 (61%)

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
6	NAG	A	782	1	-	0/6/23/26	0/1/1/1
12	A3M	A	954	-	-	0/12/19/19	0/1/1/1
6	NAG	B	769	1	-	0/6/23/26	0/1/1/1
6	NAG	B	780	1	-	0/6/23/26	0/1/1/1
12	A3M	B	955	-	-	0/12/19/19	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	955	A3M	C1-C2	2.47	1.60	1.51
6	A	782	NAG	C1-C2	2.49	1.55	1.52
12	A	954	A3M	C1-C2	2.64	1.60	1.51
12	B	955	A3M	C26-C16	4.57	1.69	1.52
12	A	954	A3M	C26-C16	4.59	1.69	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	955	A3M	C4-N3-C2	-4.58	104.27	111.39
12	A	954	A3M	C4-N3-C2	-4.39	104.57	111.39
12	A	954	A3M	O18-C14-N3	-3.41	117.40	121.66
12	A	954	A3M	C2-N3-C14	-3.10	113.58	124.08
12	B	955	A3M	C2-N3-C14	-3.10	113.58	124.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	782	NAG	8	0
12	A	954	A3M	2	0
6	B	780	NAG	4	0
12	B	955	A3M	3	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%)	-0.13	12 (1%) 73 76	14, 30, 54, 65	0
1	B	728/728 (100%)	0.03	26 (3%) 46 51	13, 31, 61, 88	0
All	All	1454/1456 (99%)	-0.05	38 (2%) 59 63	13, 31, 58, 88	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	7.0
1	B	39	SER	6.2
1	A	279	VAL	5.1
1	A	73	GLU	3.9
1	B	97	GLU	3.8

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
10	NDG	B	778	14/15	0.80	0.31	8.00	52,54,57,60	0
2	NAG	A	767	14/15	0.89	0.26	5.27	59,60,62,64	0
4	NAG	A	774	14/15	0.79	0.39	4.17	56,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	B	771	14/15	0.84	0.38	2.45	58,60,60,61	0
4	NAG	A	780	14/15	0.85	0.23	1.70	56,59,60,63	0
9	NAG	B	775	14/15	0.94	0.15	1.12	39,41,42,44	0
9	NAG	B	772	14/15	0.91	0.17	0.42	39,40,44,48	0
5	NAG	A	775	14/15	0.89	0.15	0.26	50,52,55,59	0
7	NAG	B	767	14/15	0.85	0.17	-0.70	68,69,71,72	0
2	NDG	A	768	14/15	0.67	0.38	-	65,66,67,67	0
5	MAN	A	777	11/12	0.56	0.49	-	71,72,72,73	0
9	NAG	B	776	14/15	0.90	0.16	-	46,47,49,51	0
9	BMA	B	774	11/12	0.77	0.34	-	58,59,59,59	0
5	NDG	A	776	14/15	0.70	0.35	-	63,65,66,69	0
9	BMA	B	777	11/12	0.86	0.23	-	53,54,55,55	0
8	NDG	B	770	14/15	0.89	0.25	-	50,52,54,56	0
4	NAG	A	773	14/15	0.89	0.23	-	48,49,51,54	0
3	NDG	A	770	14/15	0.74	0.51	-	70,73,77,78	0
3	NAG	A	771	14/15	0.67	0.62	-	78,80,80,80	0
9	NAG	B	773	14/15	0.83	0.31	-	51,53,54,56	0
4	NAG	A	781	14/15	0.72	0.40	-	63,65,65,66	0
10	NDG	B	779	14/15	0.75	0.55	-	62,64,65,65	0
7	FUC	B	768	10/11	0.68	0.41	-	73,73,73,73	0
2	FUC	A	769	10/11	0.91	0.31	-	63,63,63,64	0
4	NAG	A	779	14/15	0.81	0.34	-	69,70,70,70	0
3	FUC	A	772	10/11	0.76	0.57	-	79,80,80,80	0
4	NAG	A	778	14/15	0.83	0.19	-	64,65,66,67	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
6	NAG	B	780	14/15	0.80	0.36	6.04	60,62,63,63	0
12	A3M	B	955	12/12	0.95	0.17	1.13	22,23,24,24	0
12	A3M	A	954	12/12	0.95	0.15	0.91	18,19,19,19	0
11	HG	A	951	1/1	1.00	0.04	-3.24	36,36,36,36	0
11	HG	B	952	1/1	0.99	0.06	-4.48	36,36,36,36	0
11	HG	A	950	1/1	0.99	0.03	-	56,56,56,56	0
6	NAG	B	769	14/15	0.81	0.36	-	62,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	782	14/15	0.70	0.52	-	63,65,66,66	0
11	HG	B	953	1/1	0.99	0.03	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.