



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2017 – 05:18 AM EDT

PDB ID : 5A0B
Title : Crystal Structure of human neutrophil elastase in complex with a dihydropyrimidone inhibitor
Authors : vonNussbaum, F.; Li, V.M.-J.; Allerheiligen, S.; Anlauf, S.; Baerfacker, L.; Bechem, M.; Delbeck, M.; Fitzgerald, M.F.; Gerisch, M.; Gielen-Haertwig, H.; Haning, H.; Karthaus, D.; Lang, D.; Lustig, K.; Meibom, D.; Mittendorf, J.; Rosentreter, U.; Schaefer, M.; Schaefer, S.; Schamberger, J.; Telan, L.A.; Tersteegen, A.
Deposited on : 2015-04-17
Resolution : 2.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029077

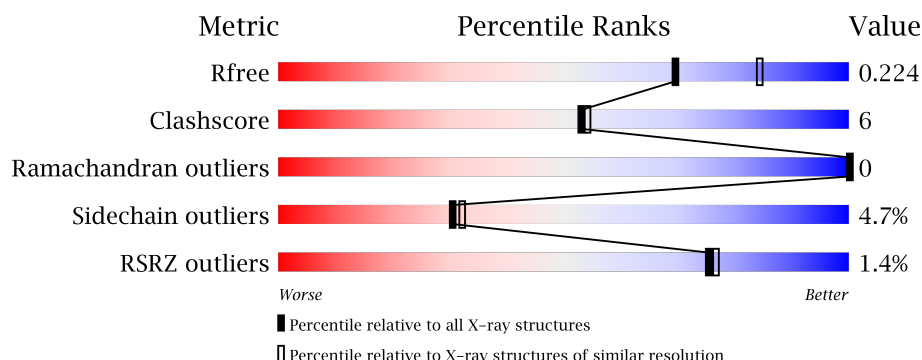
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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	218	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%; text-align: center;">84% 11% ..</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
2	NAG	A	411	-	-	-	X
5	DMS	A	1002	-	-	X	-

2 Entry composition [i](#)

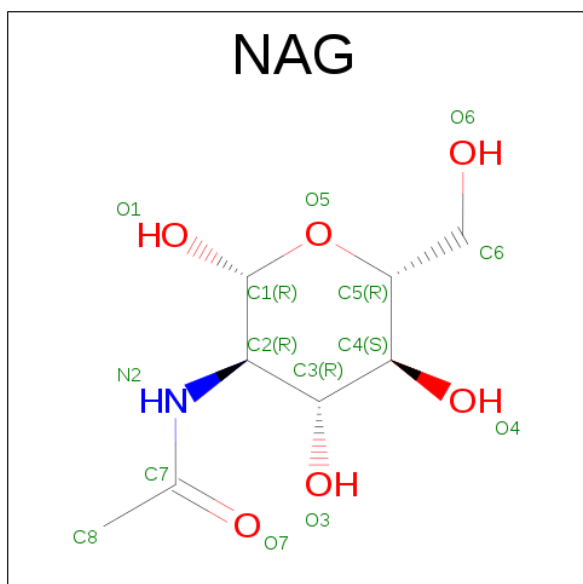
There are 6 unique types of molecules in this entry. The entry contains 1783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEUTROPHIL ELASTASE.

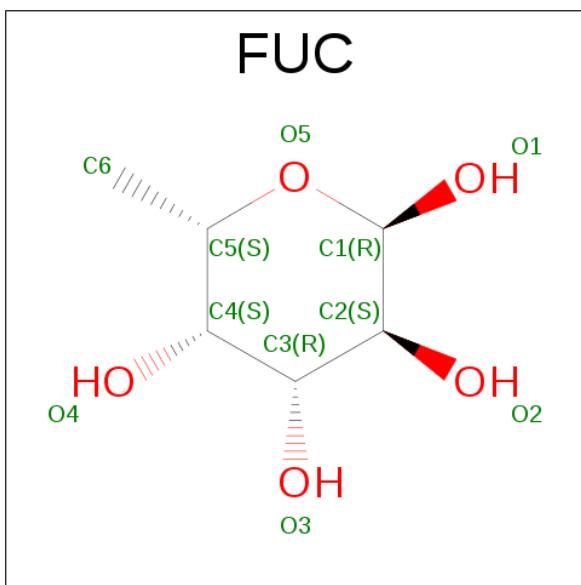
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1606	1010	306	279	11			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



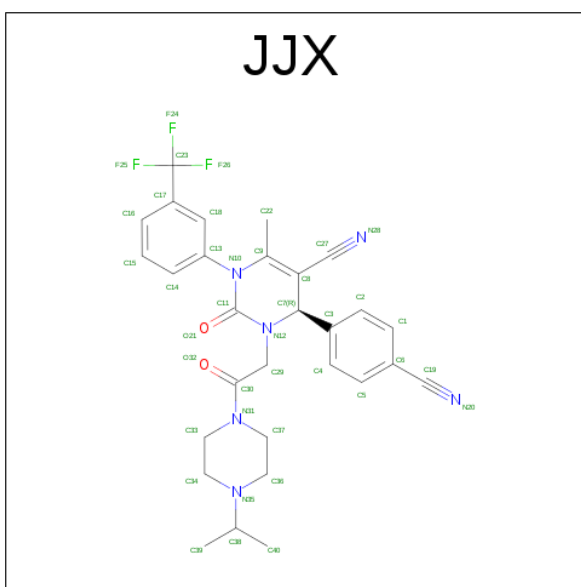
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



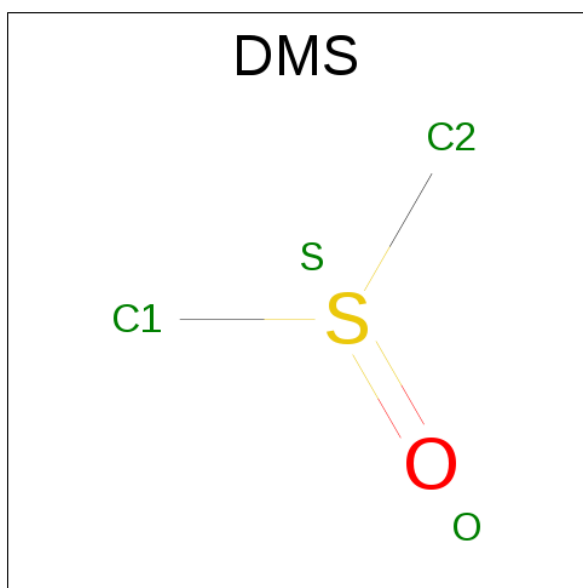
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is (4R)-4-(4-cyanophenyl)-6-methyl-2-oxidanylidene-3-[2-oxidanylidene-2-(4-propan-2-ylpiperazin-1-yl)ethyl]-1-[3-(trifluoromethyl)phenyl]-4H-pyrimidine-5-carbonitrile (three-letter code: JJX) (formula: C₂₉H₂₉F₃N₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			40	29	3	6	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

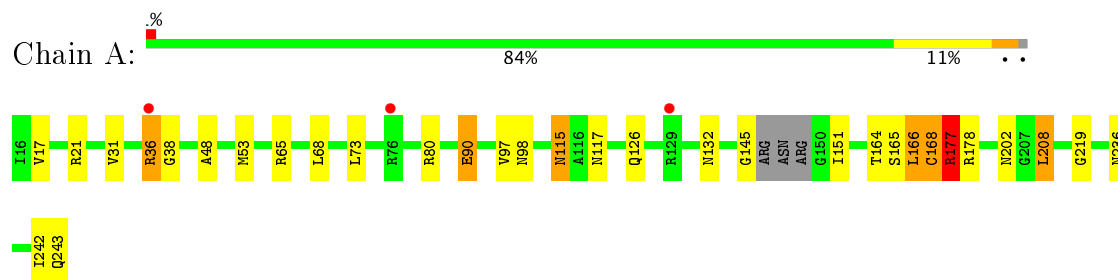
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	71	Total	O	0	0
			71	71		

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 the various outlier classes 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: NEUTROPHIL ELASTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.46 Å 77.46 Å 149.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 2.23 49.94 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.94-2.23) 99.1 (49.94-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.22 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.218 0.179 , 0.224	Depositor DCC
R_{free} test set	667 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1783	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, DMS, NAG, JJX

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	1.34	5/1635 (0.3%)	1.02	10/2221 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	ARG	C-N	26.29	1.80	1.33
1	A	202	ASN	C-N	17.43	1.64	1.33
1	A	166	LEU	C-N	10.34	1.57	1.34
1	A	168	CYS	C-N	9.07	1.54	1.34
1	A	48	ALA	CA-CB	5.03	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	O-C-N	-12.75	101.53	123.20
1	A	202	ASN	O-C-N	-9.51	107.03	123.20
1	A	36	ARG	C-N-CA	7.42	137.89	122.30
1	A	202	ASN	CA-C-N	7.24	130.68	116.20
1	A	53	MET	CG-SD-CE	-7.11	88.83	100.20
1	A	90	GLU	O-C-N	-6.93	111.61	122.70
1	A	177	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	177	ARG	NE-CZ-NH1	5.55	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	CYS	C-N-CA	-5.54	107.86	121.70
1	A	208	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	LEU	Mainchain
1	A	168	CYS	Mainchain
1	A	90	GLU	Mainchain

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	1606	0	1616	18	0
2	A	42	0	37	2	0
3	A	20	0	20	1	0
4	A	40	0	29	0	0
5	A	4	0	6	5	0
6	A	71	0	0	1	0
All	All	1783	0	1708	21	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 6.

All (21) 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:36:ARG:C	1:A:38:GLY:N	1.80	1.34
2:A:401:NAG:O4	2:A:403:NAG:C1	2.22	0.88
1:A:219:GLY:H	5:A:1002:DMS:C1	2.01	0.71
1:A:219:GLY:H	5:A:1002:DMS:H13	1.56	0.70
2:A:401:NAG:HO4	2:A:403:NAG:C1	2.04	0.68
1:A:98:ASN:O	1:A:177:ARG:NH2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1002:DMS:H11	6:A:2060:HOH:O	2.00	0.61
1:A:65:ARG:HH21	3:A:412:FUC:H2	1.66	0.61
1:A:115:ASN:ND2	1:A:117:ASN:H	2.04	0.56
1:A:115:ASN:HD22	1:A:117:ASN:H	1.53	0.55
1:A:115:ASN:C	1:A:115:ASN:HD22	2.12	0.53
1:A:36:ARG:O	1:A:38:GLY:N	2.38	0.53
1:A:242:ILE:O	1:A:243:GLN:HB2	2.13	0.48
1:A:17:VAL:HG22	1:A:145:GLY:HA2	1.95	0.48
1:A:219:GLY:N	5:A:1002:DMS:H13	2.28	0.46
1:A:73:LEU:HA	1:A:80:ARG:NH2	2.31	0.46
1:A:31:VAL:HG22	1:A:68:LEU:CD2	2.46	0.46
1:A:132:ASN:HD22	1:A:164:THR:H	1.65	0.45
1:A:126:GLN:HG2	1:A:236:ASN:ND2	2.33	0.43
1:A:219:GLY:H	5:A:1002:DMS:H12	1.80	0.43
1:A:126:GLN:HG2	1:A:236:ASN:HD21	1.85	0.41

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	211/218 (97%)	205 (97%)	6 (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	169/172 (98%)	161 (95%)	8 (5%)	30	32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	97	VAL
1	A	115	ASN
1	A	151	ILE
1	A	165	SER
1	A	177	ARG
1	A	178	ARG
1	A	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	92	ASN
1	A	115	ASN
1	A	117	ASN
1	A	119	GLN
1	A	132	ASN
1	A	233	GLN
1	A	236	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 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
4	JJX	A	1001	-	43,43,43	1.72	6 (13%)	54,63,63	1.63	13 (24%)
5	DMS	A	1002	-	3,3,3	2.67	1 (33%)	3,3,3	1.27	0
2	NAG	A	401	1,3	14,14,15	0.81	0	15,19,21	1.34	3 (20%)
3	FUC	A	402	2	9,10,11	1.26	1 (11%)	13,14,16	0.92	1 (7%)
2	NAG	A	403	-	14,14,15	0.67	0	15,19,21	1.36	1 (6%)
2	NAG	A	411	1,3	14,14,15	0.73	0	15,19,21	1.67	4 (26%)
3	FUC	A	412	2	9,10,11	1.05	0	13,14,16	1.07	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
4	JJX	A	1001	-	-	0/28/64/64	0/4/4/4
5	DMS	A	1002	-	-	0/0/0/0	0/0/0/0
2	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	402	2	-	0/0/17/20	0/1/1/1
2	NAG	A	403	-	-	0/6/23/26	0/1/1/1
2	NAG	A	411	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	412	2	-	0/0/17/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	JJX	C36-N35	2.16	1.51	1.47
4	A	1001	JJX	C23-C17	2.79	1.56	1.49
3	A	402	FUC	C2-C3	2.84	1.56	1.52
4	A	1001	JJX	C11-N12	3.02	1.41	1.37
4	A	1001	JJX	C29-C30	4.07	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	DMS	O-S	4.48	1.80	1.50
4	A	1001	JJX	C3-C7	4.68	1.58	1.52
4	A	1001	JJX	C29-N12	4.75	1.50	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	403	NAG	O5-C1-C2	-3.99	105.91	111.47
4	A	1001	JJX	O21-C11-N12	-3.98	117.21	122.12
4	A	1001	JJX	C30-C29-N12	-3.87	106.89	111.90
4	A	1001	JJX	C22-C9-C8	-3.55	119.39	124.92
2	A	411	NAG	C3-C4-C5	-3.50	104.04	110.22
4	A	1001	JJX	F24-C23-C17	-2.93	106.07	112.95
2	A	401	NAG	C2-N2-C7	-2.56	119.21	122.94
2	A	411	NAG	O5-C1-C2	-2.29	108.28	111.47
2	A	411	NAG	C1-C2-N2	-2.26	106.63	110.49
4	A	1001	JJX	O32-C30-N31	-2.15	117.77	122.05
2	A	401	NAG	C4-C3-C2	-2.09	107.96	111.02
4	A	1001	JJX	C8-C9-N10	2.08	121.57	118.89
4	A	1001	JJX	C22-C9-N10	2.24	118.91	115.65
4	A	1001	JJX	C18-C17-C23	2.28	122.79	119.58
4	A	1001	JJX	F26-C23-F25	2.28	114.14	105.70
4	A	1001	JJX	C13-N10-C11	2.44	120.26	117.11
3	A	402	FUC	C1-O5-C5	2.57	118.07	112.39
4	A	1001	JJX	C27-C8-C9	2.60	121.81	119.75
2	A	401	NAG	C1-C2-N2	2.63	114.98	110.49
2	A	411	NAG	O4-C4-C5	2.67	116.02	109.28
4	A	1001	JJX	C14-C13-N10	3.39	123.76	119.63
4	A	1001	JJX	C29-C30-N31	3.66	121.91	117.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	DMS	5	0
2	A	401	NAG	2	0
2	A	403	NAG	2	0
3	A	412	FUC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:ARG	C	38:GLY	N	1.80
1	A	202:ASN	C	207:GLY	N	1.64

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	215/218 (98%)	-0.22	3 (1%) 75 77	14, 22, 37, 52	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	ARG	4.3
1	A	36	ARG	3.1
1	A	129	ARG	2.8

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](#)

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
2	NAG	A	411	14/15	0.91	0.19	2.94	29,36,49,49	0
3	FUC	A	402	10/11	0.95	0.15	0.22	22,25,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	JJX	A	1001	40/40	0.96	0.11	0.02	15,20,32,35	0
2	NAG	A	401	14/15	0.95	0.23	-	31,33,42,42	0
2	NAG	A	403	14/15	0.81	0.33	-	44,54,59,59	0
5	DMS	A	1002	4/4	0.92	0.17	-	52,54,54,56	0
3	FUC	A	412	10/11	0.81	0.28	-	29,37,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.