



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM GMT

PDB ID : 3QBJ
Title : Crystal structure of dipeptidyl peptidase IV in complex with inhibitor
Authors : Liu, S.P.
Deposited on : 2011-01-13
Resolution : 2.21 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 (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

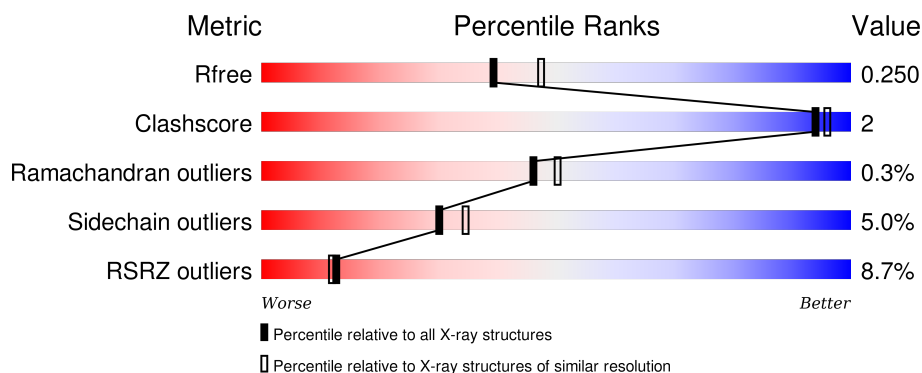
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	748	<div> <div>9%</div> <div>89%</div> <div>8%</div> </div>
1	B	748	<div> <div>8%</div> <div>89%</div> <div>8%</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
4	NAG	A	800	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12183 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ALA	ASN	ENGINEERED MUTATION	UNP P27487
A	520	ALA	ASN	ENGINEERED MUTATION	UNP P27487
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
A	774	HIS	-	EXPRESSION TAG	UNP P27487
A	775	HIS	-	EXPRESSION TAG	UNP P27487
A	776	HIS	-	EXPRESSION TAG	UNP P27487
A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
B	150	ALA	ASN	ENGINEERED MUTATION	UNP P27487
B	520	ALA	ASN	ENGINEERED MUTATION	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487

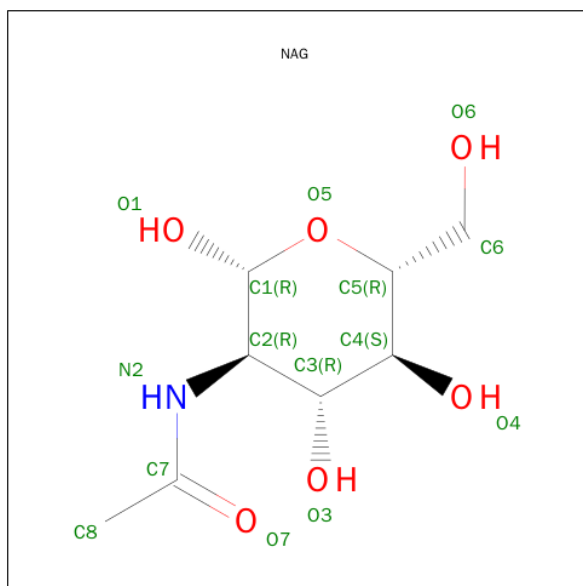
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



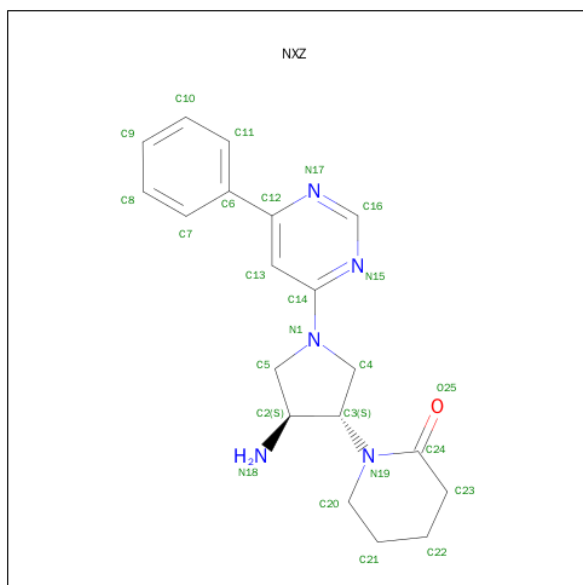
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 1-[(3S,4S)-4-AMINO-1-(6-PHENYLPYRIMIDIN-4-YL)PYRROLIDIN-3-YL] PIPERIDIN-2-ONE (three-letter code: NXZ) (formula: C₁₉H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	19	5	1		
5	B	1	Total	C	N	O	0	0
			25	19	5	1		

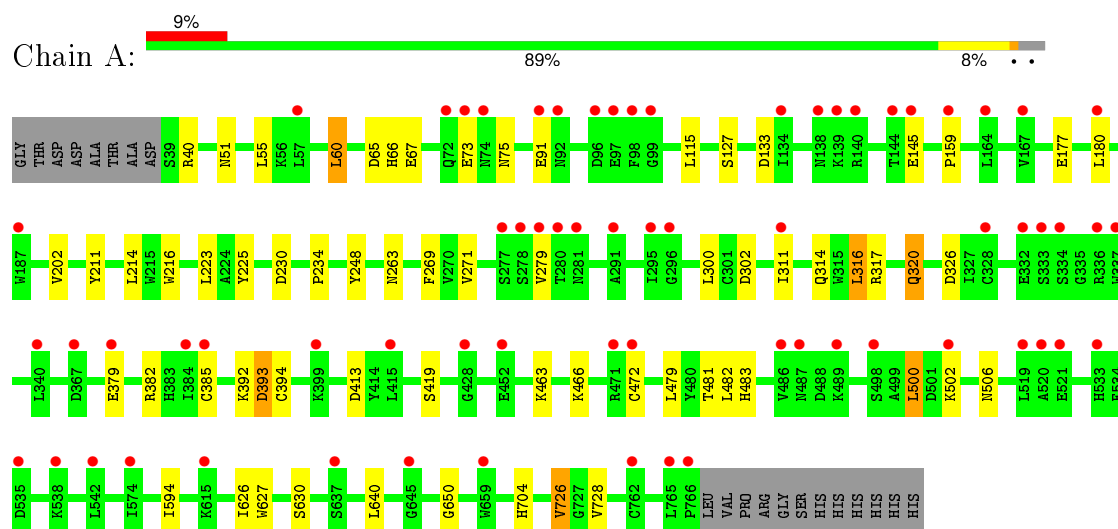
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	43	Total	O	0	0
			43	43		

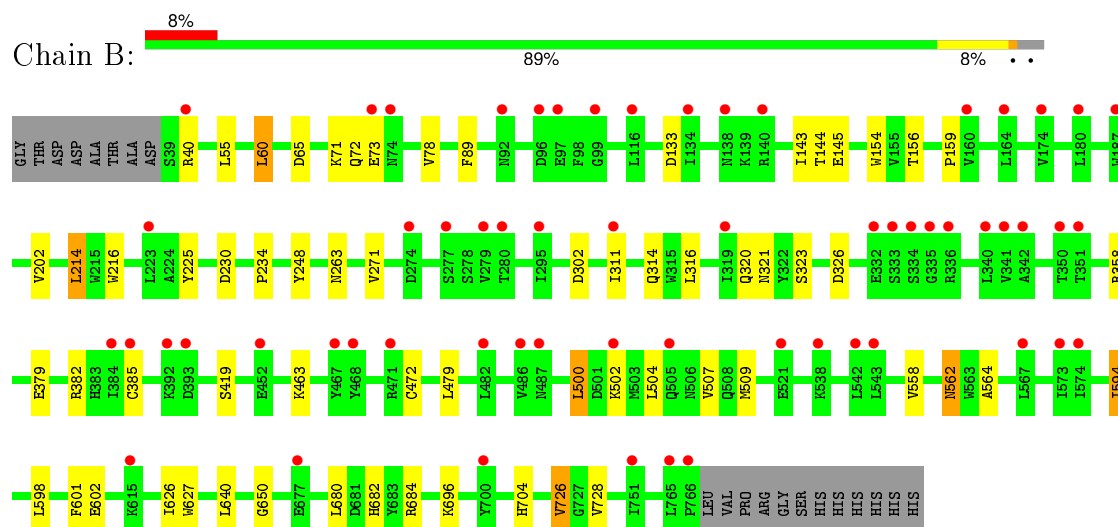
3 Residue-property plots [i](#)

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 4



- Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.75Å 69.08Å 424.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.11 – 2.21 18.09 – 2.21	Depositor EDS
% Data completeness (in resolution range)	80.3 (18.11-2.21) 80.3 (18.09-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.21Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.202 , 0.235 0.215 , 0.250	Depositor DCC
R_{free} test set	3918 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.962	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.5	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	8 of 78758 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: NXZ, BMA, NAG, 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	0.50	0/6129	0.70	1/8336 (0.0%)
1	B	0.50	0/6129	0.70	1/8336 (0.0%)
All	All	0.50	0/12258	0.70	2/16672 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	60	LEU	CA-CB-CG	5.08	126.98	115.30

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	5957	0	5678	23	0
1	B	5957	0	5681	22	0
2	A	28	0	25	0	0
2	B	28	0	25	0	0
3	A	50	0	43	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	25	0	23	0	0
5	B	25	0	23	0	0
6	A	28	0	0	0	0
6	B	43	0	0	1	0
All	All	12183	0	11537	43	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 2.

All (43) 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:B:78:VAL:HG23	1:B:89:PHE:HB2	1.73	0.69
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.75	0.69
1:A:225:TYR:CE1	1:A:269:PHE:HD1	2.11	0.68
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.76	0.67
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.29	0.65
1:B:696:LYS:HG2	1:B:728:VAL:HG22	1.78	0.65
1:B:316:LEU:HD13	1:B:323:SER:HB3	1.81	0.62
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.69	0.58
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.87	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.88	0.56
1:B:626:ILE:O	1:B:650:GLY:HA2	2.06	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.88	0.56
1:A:626:ILE:O	1:A:650:GLY:HA2	2.06	0.55
1:A:214:LEU:HD22	1:A:223:LEU:HD11	1.91	0.51
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.92	0.51
1:B:598:LEU:O	1:B:682:HIS:HE1	1.94	0.51
1:A:316:LEU:HD21	1:A:320:GLN:HA	1.92	0.51
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.93	0.50
1:A:316:LEU:CD2	1:A:320:GLN:HA	2.43	0.49
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.95	0.49
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.95	0.48
1:B:65:ASP:OD1	1:B:463:LYS:O	2.31	0.48
1:B:594:ILE:HD11	1:B:602:GLU:H	1.79	0.47
1:A:65:ASP:HB3	1:A:463:LYS:O	2.15	0.47
1:B:214:LEU:HD12	1:B:225:TYR:HB3	1.97	0.46
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.96	0.46
1:B:214:LEU:CD1	1:B:225:TYR:HB3	2.47	0.45
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.98	0.45
1:A:393:ASP:HB2	1:A:394:CYS:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.98	0.44
1:A:316:LEU:HD22	1:A:317:ARG:O	2.19	0.43
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.54	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.54	0.42
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.55	0.42
1:A:177:GLU:CB	1:A:180:LEU:HD23	2.49	0.41
1:A:55:LEU:HD23	1:A:500:LEU:HD12	2.01	0.41
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.03	0.41
1:A:66:HIS:HD2	1:A:67:GLU:HG3	1.86	0.41
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.56	0.41
1:A:75:ASN:HD22	1:A:91:GLU:HA	1.85	0.41
1:B:358:ARG:HD2	6:B:802:HOH:O	2.21	0.41
1:B:594:ILE:HD12	1:B:601:PHE:HB2	2.03	0.40
1:B:55:LEU:HD23	1:B:500:LEU:HD12	2.02	0.40

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	726/748 (97%)	692 (95%)	31 (4%)	3 (0%)	39	41
1	B	726/748 (97%)	694 (96%)	30 (4%)	2 (0%)	46	50
All	All	1452/1496 (97%)	1386 (96%)	61 (4%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	73	GLU
1	A	320	GLN
1	A	392	LYS

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Mol	Chain	Res	Type
1	B	320	GLN

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	651/667 (98%)	618 (95%)	33 (5%)	29	33
1	B	651/667 (98%)	619 (95%)	32 (5%)	31	35
All	All	1302/1334 (98%)	1237 (95%)	65 (5%)	30	34

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	51	ASN
1	A	60	LEU
1	A	115	LEU
1	A	133	ASP
1	A	145	GLU
1	A	202	VAL
1	A	230	ASP
1	A	263	ASN
1	A	271	VAL
1	A	279	VAL
1	A	300	LEU
1	A	311	ILE
1	A	316	LEU
1	A	326	ASP
1	A	379	GLU
1	A	382	ARG
1	A	385	CYS
1	A	393	ASP
1	A	413	ASP
1	A	419	SER
1	A	466	LYS

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Mol	Chain	Res	Type
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	LYS
1	A	506	ASN
1	A	594	ILE
1	A	627	TRP
1	A	630	SER
1	A	704	HIS
1	A	726	VAL
1	B	40	ARG
1	B	60	LEU
1	B	71	LYS
1	B	72	GLN
1	B	133	ASP
1	B	143	ILE
1	B	144	THR
1	B	145	GLU
1	B	202	VAL
1	B	214	LEU
1	B	230	ASP
1	B	263	ASN
1	B	271	VAL
1	B	311	ILE
1	B	321	ASN
1	B	326	ASP
1	B	379	GLU
1	B	382	ARG
1	B	385	CYS
1	B	419	SER
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	502	LYS
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	627	TRP
1	B	680	LEU
1	B	684	ARG
1	B	704	HIS

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Mol	Chain	Res	Type
1	B	726	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	75	ASN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	363	HIS
1	A	435	GLN
1	A	483	HIS
1	A	697	GLN
1	B	75	ASN
1	B	263	ASN
1	B	298	HIS
1	B	321	ASN
1	B	383	HIS
1	B	562	ASN
1	B	586	GLN
1	B	682	HIS
1	B	731	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

8 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	794	1,2	14,14,15	1.45	2 (14%)	15,19,21	1.65	3 (20%)
3	NAG	A	796	1,3	14,14,15	0.97	0	15,19,21	1.35	1 (6%)
2	NAG	A	797	2	14,14,15	1.78	2 (14%)	15,19,21	2.15	1 (6%)
3	NAG	A	798	3	14,14,15	1.99	4 (28%)	15,19,21	1.86	4 (26%)
3	BMA	A	802	3	11,11,12	1.99	3 (27%)	14,15,17	2.39	6 (42%)
3	MAN	A	803	3	11,11,12	1.73	2 (18%)	14,15,17	1.50	3 (21%)
2	NAG	B	794	1,2	14,14,15	1.47	3 (21%)	15,19,21	0.89	0
2	NAG	B	797	2	14,14,15	1.43	3 (21%)	15,19,21	2.03	3 (20%)

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	794	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	796	1,3	-	0/6/23/26	0/1/1/1
2	NAG	A	797	2	-	0/6/23/26	0/1/1/1
3	NAG	A	798	3	-	0/6/23/26	0/1/1/1
3	BMA	A	802	3	-	0/2/19/22	0/1/1/1
3	MAN	A	803	3	-	0/2/19/22	0/1/1/1
2	NAG	B	794	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	797	2	-	0/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	794	NAG	C2-N2	-2.59	1.41	1.46
2	B	794	NAG	O5-C1	-2.47	1.39	1.43
2	B	794	NAG	C4-C5	2.03	1.57	1.53
2	B	797	NAG	C3-C2	2.06	1.57	1.52
2	B	797	NAG	C1-C2	2.20	1.55	1.52
3	A	802	BMA	C4-C3	2.28	1.58	1.52
2	B	797	NAG	O4-C4	2.33	1.48	1.43
2	B	794	NAG	C1-C2	2.37	1.55	1.52
2	A	797	NAG	O5-C5	2.39	1.48	1.43
3	A	798	NAG	C2-N2	2.72	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	BMA	C4-C5	3.05	1.59	1.53
3	A	803	MAN	C1-C2	3.15	1.59	1.52
3	A	798	NAG	C4-C3	3.17	1.60	1.52
3	A	798	NAG	C1-C2	3.28	1.57	1.52
3	A	803	MAN	C2-C3	3.34	1.57	1.52
2	A	794	NAG	C1-C2	3.46	1.57	1.52
3	A	802	BMA	C2-C3	3.80	1.57	1.52
3	A	798	NAG	C3-C2	3.85	1.61	1.52
2	A	797	NAG	C1-C2	4.55	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	BMA	C1-C2-C3	-4.25	104.52	109.54
2	A	794	NAG	C3-C4-C5	-3.16	104.68	110.20
2	A	794	NAG	C8-C7-N2	-2.84	110.66	116.11
3	A	803	MAN	O4-C4-C3	-2.70	104.25	110.34
3	A	798	NAG	O4-C4-C3	-2.41	104.90	110.34
3	A	802	BMA	O4-C4-C3	-2.33	105.08	110.34
3	A	796	NAG	O4-C4-C3	-2.32	105.12	110.34
2	B	797	NAG	C8-C7-N2	-2.27	111.75	116.11
2	B	797	NAG	O5-C5-C6	2.01	111.71	107.35
3	A	803	MAN	C1-C2-C3	2.15	112.09	109.54
3	A	803	MAN	C2-C3-C4	2.21	114.80	111.04
2	A	794	NAG	C2-N2-C7	2.33	126.03	123.04
3	A	802	BMA	C3-C4-C5	2.45	114.48	110.20
3	A	802	BMA	O3-C3-C2	2.69	114.86	110.00
3	A	798	NAG	C3-C2-N2	2.70	117.03	110.56
3	A	798	NAG	C3-C4-C5	3.50	116.29	110.20
3	A	802	BMA	O2-C2-C3	3.59	117.33	110.12
3	A	802	BMA	C2-C3-C4	4.37	118.46	111.04
3	A	798	NAG	C4-C3-C2	4.62	118.41	111.23
2	B	797	NAG	C1-O5-C5	6.88	120.98	112.25
2	A	797	NAG	C1-O5-C5	7.22	121.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

5 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	NAG	A	799	1	14,14,15	1.81	2 (14%)	15,19,21	2.64	5 (33%)
4	NAG	A	800	1	14,14,15	2.18	5 (35%)	15,19,21	2.10	3 (20%)
5	NXZ	A	900	-	28,28,28	2.17	13 (46%)	31,39,39	3.49	11 (35%)
4	NAG	B	796	1	14,14,15	1.17	2 (14%)	15,19,21	1.10	1 (6%)
5	NXZ	B	900	-	28,28,28	2.40	13 (46%)	31,39,39	3.32	10 (32%)

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	799	1	-	0/6/23/26	0/1/1/1
4	NAG	A	800	1	-	0/6/23/26	0/1/1/1
5	NXZ	A	900	-	-	0/11/35/35	0/4/4/4
4	NAG	B	796	1	-	0/6/23/26	0/1/1/1
5	NXZ	B	900	-	-	0/11/35/35	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	NXZ	C24-N19	2.05	1.38	1.35
5	A	900	NXZ	C4-N1	2.07	1.49	1.46
5	B	900	NXZ	C21-C22	2.14	1.60	1.51
4	A	800	NAG	C2-N2	2.18	1.50	1.46
4	B	796	NAG	C3-C2	2.21	1.57	1.52
5	A	900	NXZ	C9-C10	2.37	1.44	1.38
4	A	799	NAG	C4-C5	2.37	1.58	1.53
4	A	800	NAG	O4-C4	2.50	1.48	1.43
5	A	900	NXZ	C8-C7	2.51	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	NXZ	C13-C12	2.53	1.43	1.39
5	B	900	NXZ	C8-C7	2.55	1.44	1.38
5	A	900	NXZ	C20-N19	2.67	1.50	1.47
5	A	900	NXZ	C12-N17	2.70	1.40	1.35
5	B	900	NXZ	C10-C11	2.72	1.44	1.38
4	B	796	NAG	C1-C2	2.78	1.56	1.52
5	B	900	NXZ	C5-C2	2.79	1.57	1.52
5	A	900	NXZ	C10-C11	2.83	1.44	1.38
5	A	900	NXZ	C8-C9	2.91	1.45	1.38
5	B	900	NXZ	C13-C12	3.00	1.44	1.39
5	A	900	NXZ	C5-N1	3.03	1.50	1.46
5	B	900	NXZ	C24-N19	3.03	1.40	1.35
5	B	900	NXZ	C4-N1	3.03	1.50	1.46
4	A	800	NAG	C4-C3	3.19	1.60	1.52
5	B	900	NXZ	C11-C6	3.22	1.46	1.39
5	B	900	NXZ	C9-C10	3.35	1.46	1.38
5	B	900	NXZ	C12-N17	3.35	1.42	1.35
4	A	800	NAG	C3-C2	3.35	1.60	1.52
5	A	900	NXZ	C11-C6	3.40	1.46	1.39
5	A	900	NXZ	C14-N15	3.66	1.42	1.34
4	A	799	NAG	C1-C2	3.67	1.57	1.52
5	B	900	NXZ	C20-N19	4.12	1.52	1.47
5	B	900	NXZ	C7-C6	4.32	1.48	1.39
5	B	900	NXZ	C14-N15	4.53	1.43	1.34
5	A	900	NXZ	C7-C6	4.63	1.49	1.39
4	A	800	NAG	C1-C2	4.78	1.59	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	900	NXZ	N17-C16-N15	-7.66	115.76	128.67
5	B	900	NXZ	N17-C16-N15	-7.03	116.81	128.67
5	B	900	NXZ	C3-C4-N1	-4.26	95.98	102.96
4	A	799	NAG	C4-C3-C2	-3.99	105.03	111.23
5	A	900	NXZ	C3-C4-N1	-3.92	96.53	102.96
5	B	900	NXZ	C2-C5-N1	-2.62	98.67	103.06
5	B	900	NXZ	C13-C14-N15	-2.48	118.05	122.49
5	B	900	NXZ	C4-N1-C14	-2.47	116.98	123.52
5	A	900	NXZ	C13-C14-N15	-2.40	118.20	122.49
5	A	900	NXZ	C2-C5-N1	-2.33	99.15	103.06
5	A	900	NXZ	C8-C7-C6	-2.07	117.81	120.56
5	A	900	NXZ	C4-N1-C14	-2.07	118.04	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	900	NXZ	C22-C21-C20	2.08	115.37	111.26
4	B	796	NAG	C4-C3-C2	2.14	114.55	111.23
4	A	799	NAG	O3-C3-C2	2.26	113.59	109.11
5	B	900	NXZ	C10-C9-C8	2.27	123.92	119.93
4	A	800	NAG	O4-C4-C3	2.37	115.67	110.34
5	A	900	NXZ	C5-N1-C4	2.41	117.53	112.42
5	A	900	NXZ	C21-C20-N19	2.72	114.91	110.71
5	B	900	NXZ	C5-N1-C4	2.90	118.57	112.42
4	A	799	NAG	O3-C3-C4	3.22	117.59	110.34
5	B	900	NXZ	C21-C20-N19	3.24	115.72	110.71
4	A	799	NAG	C3-C2-N2	3.52	118.99	110.56
4	A	800	NAG	C3-C2-N2	4.72	121.86	110.56
4	A	800	NAG	C1-O5-C5	4.79	118.33	112.25
5	B	900	NXZ	C16-N17-C12	5.09	122.90	115.74
5	A	900	NXZ	C16-N17-C12	5.96	124.11	115.74
4	A	799	NAG	C1-O5-C5	7.17	121.34	112.25
5	B	900	NXZ	C16-N15-C14	13.48	125.19	114.84
5	A	900	NXZ	C16-N15-C14	14.42	125.92	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/748 (97%)	0.50	67 (9%) 11 10	50, 72, 105, 128	0
1	B	728/748 (97%)	0.42	60 (8%) 14 13	46, 66, 99, 124	0
All	All	1456/1496 (97%)	0.46	127 (8%) 13 12	46, 69, 102, 128	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	7.1
1	A	279	VAL	6.8
1	B	280	THR	6.5
1	A	280	THR	5.4
1	A	97	GLU	4.6
1	A	615	LYS	4.5
1	A	73	GLU	4.5
1	A	278	SER	4.4
1	B	333	SER	4.4
1	B	542	LEU	4.3
1	A	72	GLN	4.3
1	A	520	ALA	4.3
1	B	574	ILE	4.3
1	B	766	PRO	4.2
1	A	766	PRO	4.1
1	B	97	GLU	4.1
1	A	144	THR	4.0
1	B	332	GLU	4.0
1	A	99	GLY	4.0
1	A	487	ASN	4.0
1	A	296	GLY	3.9
1	B	521	GLU	3.9
1	A	333	SER	3.9
1	B	341	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	3.7
1	B	138	ASN	3.7
1	B	73	GLU	3.6
1	B	393	ASP	3.6
1	B	335	GLY	3.6
1	B	615	LYS	3.6
1	B	74	ASN	3.5
1	B	392	LYS	3.5
1	A	134	ILE	3.5
1	B	342	ALA	3.5
1	A	138	ASN	3.4
1	A	574	ILE	3.4
1	A	765	LEU	3.3
1	B	134	ILE	3.3
1	A	74	ASN	3.3
1	B	486	VAL	3.3
1	B	350	THR	3.2
1	A	180	LEU	3.1
1	A	277	SER	3.1
1	A	291	ALA	3.1
1	B	336	ARG	3.1
1	A	96	ASP	3.1
1	A	542	LEU	3.1
1	B	96	ASP	3.0
1	A	452	GLU	3.0
1	B	538	LYS	3.0
1	B	384	ILE	2.9
1	B	487	ASN	2.9
1	A	533	HIS	2.9
1	A	139	LYS	2.9
1	A	159	PRO	2.8
1	A	471	ARG	2.8
1	B	351	THR	2.8
1	B	502	LYS	2.8
1	A	295	ILE	2.8
1	A	486	VAL	2.8
1	A	337	TRP	2.8
1	A	167	VAL	2.7
1	A	334	SER	2.7
1	A	140	ARG	2.7
1	A	311	ILE	2.6
1	A	659	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	336	ARG	2.6
1	B	140	ARG	2.6
1	A	399	LYS	2.6
1	A	521	GLU	2.6
1	A	332	GLU	2.6
1	B	92	ASN	2.6
1	A	281	ASN	2.5
1	A	384	ILE	2.5
1	B	319	ILE	2.5
1	A	340	LEU	2.4
1	A	367	ASP	2.4
1	B	751	ILE	2.4
1	B	334	SER	2.4
1	B	471	ARG	2.4
1	B	223	LEU	2.4
1	B	40	ARG	2.4
1	A	498	SER	2.4
1	B	277	SER	2.4
1	A	538	LYS	2.4
1	A	502	LYS	2.4
1	B	567	LEU	2.4
1	B	452	GLU	2.3
1	B	295	ILE	2.3
1	B	160	VAL	2.3
1	B	573	ILE	2.3
1	A	489	LYS	2.3
1	A	385	CYS	2.3
1	A	762	CYS	2.3
1	B	385	CYS	2.3
1	B	274	ASP	2.3
1	B	467	TYR	2.3
1	B	164	LEU	2.3
1	A	472	CYS	2.2
1	B	677	GLU	2.2
1	B	187	TRP	2.2
1	A	535	ASP	2.2
1	B	311	ILE	2.2
1	A	415	LEU	2.2
1	B	174	VAL	2.1
1	A	328	CYS	2.1
1	A	379	GLU	2.1
1	A	92	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	PHE	2.1
1	B	700	TYR	2.1
1	A	164	LEU	2.1
1	B	543	LEU	2.1
1	A	187	TRP	2.1
1	A	91	GLU	2.1
1	A	428	GLY	2.1
1	A	519	LEU	2.1
1	A	645	GLY	2.0
1	A	57	LEU	2.0
1	B	468	TYR	2.0
1	A	637	SER	2.0
1	B	99	GLY	2.0
1	B	116	LEU	2.0
1	B	180	LEU	2.0
1	A	145	GLU	2.0
1	B	505	GLN	2.0
1	B	482	LEU	2.0
1	B	765	LEU	2.0

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
2	NAG	B	794	14/15	0.94	0.14	0.24	63,66,72,72	0
3	NAG	A	796	14/15	0.90	0.16	0.20	68,74,77,78	0
2	NAG	A	794	14/15	0.93	0.10	-0.57	75,79,84,85	0
3	NAG	A	798	14/15	0.83	0.35	-	77,81,83,83	0
3	BMA	A	802	11/12	0.77	0.30	-	96,99,101,102	0
3	MAN	A	803	11/12	0.78	0.39	-	106,108,111,112	0
2	NAG	B	797	14/15	0.87	0.35	-	94,98,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	797	14/15	0.92	0.34	-	87,91,94,94	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
4	NAG	A	800	14/15	0.83	0.34	4.51	89,93,95,95	0
4	NAG	B	796	14/15	0.85	0.23	1.44	70,76,80,81	0
5	NXZ	A	900	25/25	0.84	0.17	0.52	46,54,76,78	0
5	NXZ	B	900	25/25	0.88	0.14	-0.10	41,49,69,70	0
4	NAG	A	799	14/15	0.77	0.38	-	99,103,105,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.