



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 01:20 AM BST

PDB ID : 5X2P
Title : Crystal structure of the medaka fish taste receptor T1r2a-T1r3 ligand binding domains in complex with L-glutamate
Authors : Nuemket, N.; Yasui, N.; Atsumi, N.; Yamashita, A.
Deposited on : 2017-02-02
Resolution : 2.61 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

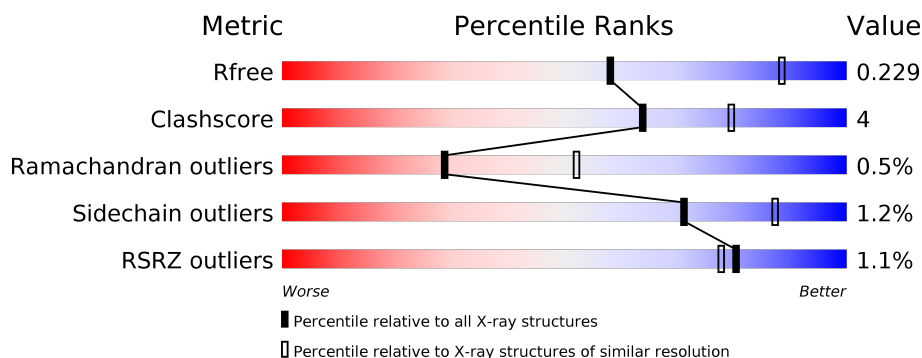
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. 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	461	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>
1	C	461	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
2	B	478	<div> <div></div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
2	D	478	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
3	H	225	<div> <div></div> <div> <div></div> <div>89%</div> <div>8%</div> <div>•</div> </div> </div>
3	J	225	<div> <div></div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	K	217	 87% 12%
4	L	217	 90% 10%
5	E	3	 67% 33%
6	F	2	 50% 50%

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
7	NAG	B	908	-	-	-	X
7	NAG	C	902	-	-	-	X
7	NAG	D	905	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21069 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 Taste receptor, type 1, member 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3387	2189	561	621	16			
1	C	430	Total	C	N	O	S	0	1	0
			3407	2198	565	626	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP A0A173M0G2
A	476	GLY	-	expression tag	UNP A0A173M0G2
A	477	ILE	-	expression tag	UNP A0A173M0G2
A	478	GLU	-	expression tag	UNP A0A173M0G2
A	479	GLY	-	expression tag	UNP A0A173M0G2
A	480	ARG	-	expression tag	UNP A0A173M0G2
C	475	SER	-	expression tag	UNP A0A173M0G2
C	476	GLY	-	expression tag	UNP A0A173M0G2
C	477	ILE	-	expression tag	UNP A0A173M0G2
C	478	GLU	-	expression tag	UNP A0A173M0G2
C	479	GLY	-	expression tag	UNP A0A173M0G2
C	480	ARG	-	expression tag	UNP A0A173M0G2

- Molecule 2 is a protein called Taste receptor, type 1, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	453	Total	C	N	O	S	0	0	0
			3551	2282	571	683	15			
2	D	414	Total	C	N	O	S	0	0	0
			3211	2060	520	618	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	492	SER	-	expression tag	UNP A0A173M094
B	493	GLY	-	expression tag	UNP A0A173M094
B	494	ILE	-	expression tag	UNP A0A173M094
B	495	GLU	-	expression tag	UNP A0A173M094
B	496	GLY	-	expression tag	UNP A0A173M094
B	497	ARG	-	expression tag	UNP A0A173M094
D	492	SER	-	expression tag	UNP A0A173M094
D	493	GLY	-	expression tag	UNP A0A173M094
D	494	ILE	-	expression tag	UNP A0A173M094
D	495	GLU	-	expression tag	UNP A0A173M094
D	496	GLY	-	expression tag	UNP A0A173M094
D	497	ARG	-	expression tag	UNP A0A173M094

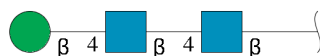
- Molecule 3 is a protein called Fab16A Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	0	0
			1662	1056	274	324	8			
3	J	218	Total	C	N	O	S	0	0	0
			1651	1050	272	321	8			

- Molecule 4 is a protein called Fab16A Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	217	Total	C	N	O	S	0	0	0
			1679	1040	288	345	6			
4	K	216	Total	C	N	O	S	0	0	0
			1670	1035	287	342	6			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



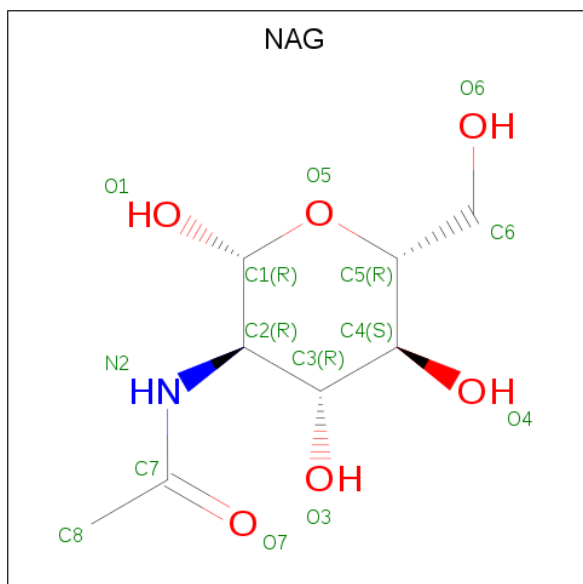
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



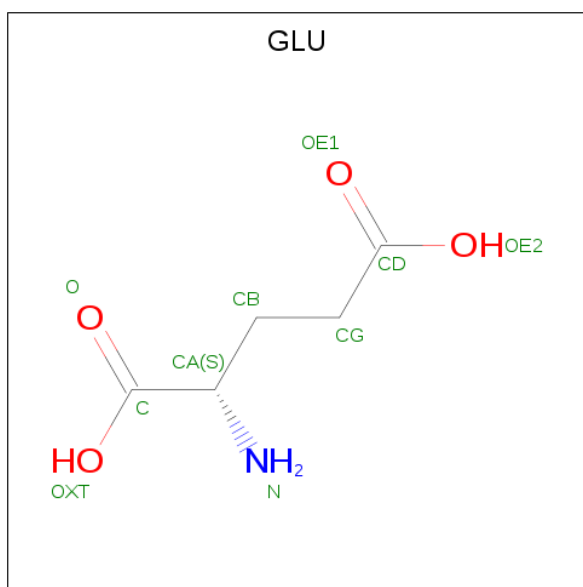
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			10	5	1	4		
8	B	1	Total	C	N	O	0	0
			10	5	1	4		
8	C	1	Total	C	N	O	0	0
			10	5	1	4		
8	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		
10	D	1	Total	Cl	0	0
			1	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	K	1	Total Ca 1 1	0	0

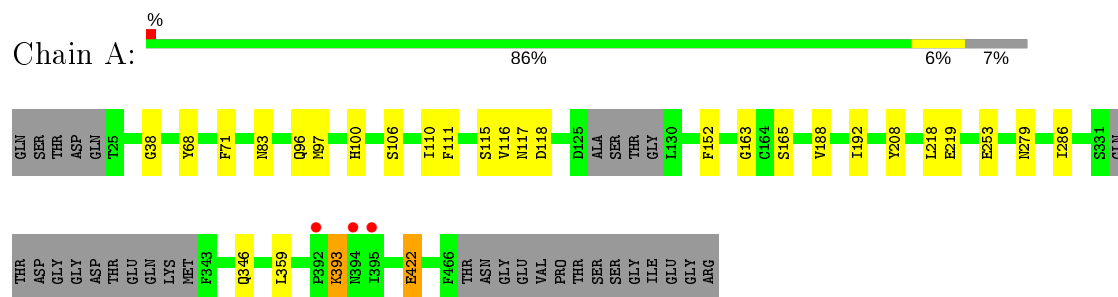
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	81	Total O 81 81	0	0
12	B	56	Total O 56 56	0	0
12	C	83	Total O 83 83	0	0
12	D	33	Total O 33 33	0	0
12	H	42	Total O 42 42	0	0
12	L	46	Total O 46 46	0	0
12	J	21	Total O 21 21	0	0
12	K	55	Total O 55 55	0	0

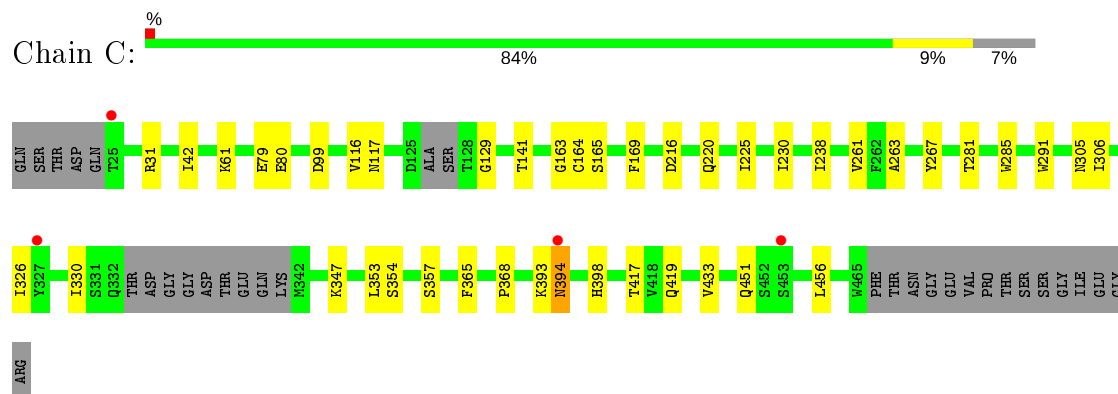
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

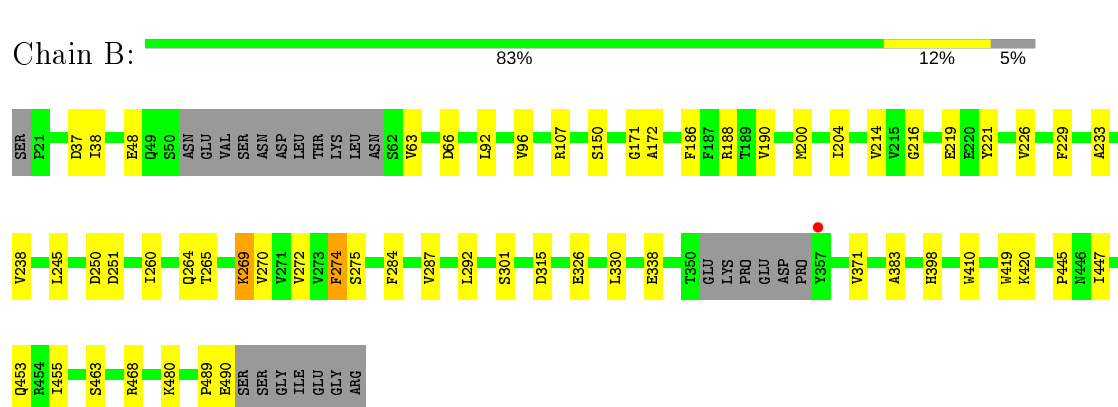
- Molecule 1: Taste receptor, type 1, member 2a



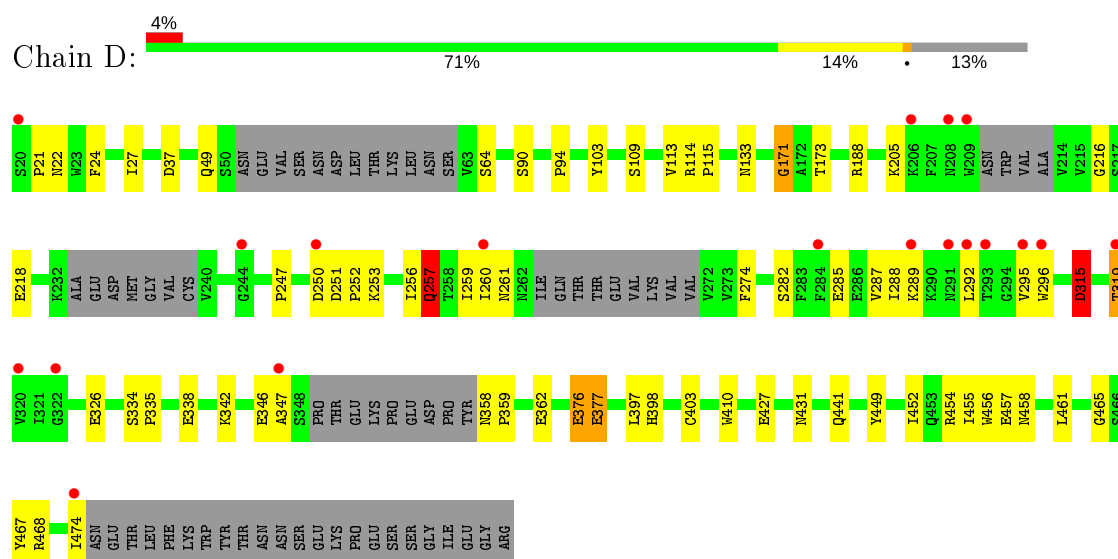
- Molecule 1: Taste receptor, type 1, member 2a



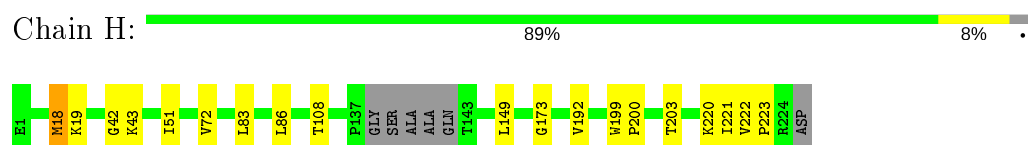
- Molecule 2: Taste receptor, type 1, member 3



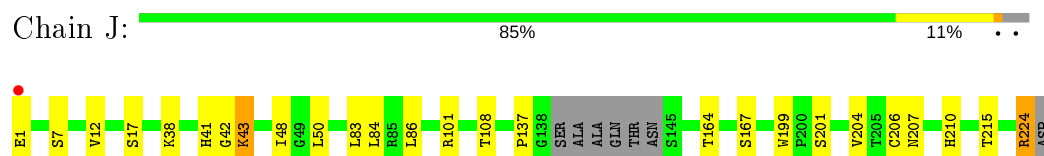
- Molecule 2: Taste receptor, type 1, member 3



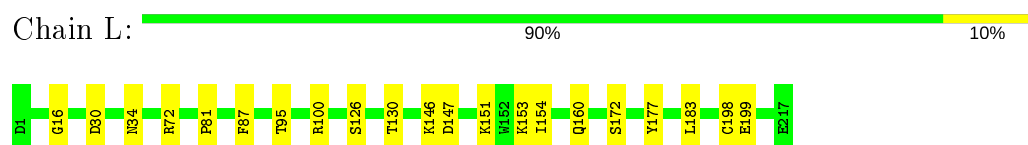
- Molecule 3: Fab16A Heavy chain



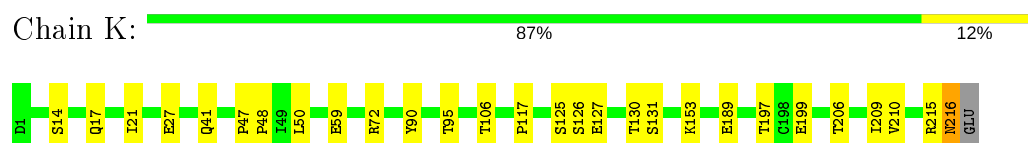
- Molecule 3: Fab16A Heavy chain



- Molecule 4: Fab16A Light chain



- Molecule 4: Fab16A Light chain



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.63Å 116.06Å 129.59Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.14 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.61) 95.7 (50.14-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.153 , 0.228 0.155 , 0.229	Depositor DCC
R_{free} test set	4297 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21069	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: NA, CA, BMA, NAG, CL

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	0.46	0/3475	0.58	0/4720
1	C	0.45	0/3497	0.57	0/4749
2	B	0.43	0/3633	0.56	1/4941 (0.0%)
2	D	0.42	0/3281	0.57	0/4456
3	H	0.43	0/1706	0.60	0/2331
3	J	0.40	0/1695	0.58	1/2315 (0.0%)
4	K	0.44	0/1707	0.57	0/2320
4	L	0.48	1/1716 (0.1%)	0.59	0/2332
All	All	0.44	1/20710 (0.0%)	0.57	2/28164 (0.0%)

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	C	0	1
2	D	0	2
3	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	198	CYS	CB-SG	-5.29	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	LYS	CA-CB-CG	-5.62	101.03	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	50	LEU	CA-CB-CG	5.24	127.36	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	451	GLN	Peptide
2	D	257	GLN	Peptide
2	D	315	ASP	Peptide
3	J	42	GLY	Peptide

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	3387	0	3308	21	0
1	C	3407	0	3331	26	0
2	B	3551	0	3504	33	0
2	D	3211	0	3143	46	0
3	H	1662	0	1642	11	0
3	J	1651	0	1632	14	0
4	K	1670	0	1596	15	0
4	L	1679	0	1602	10	0
5	E	39	0	34	0	0
6	F	28	0	25	1	0
7	A	98	0	91	2	0
7	B	84	0	78	1	0
7	C	98	0	91	2	0
7	D	42	0	39	0	0
8	A	10	0	5	1	0
8	B	10	0	5	1	0
8	C	10	0	5	1	0
8	D	10	0	5	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1	0	0	0	0
12	A	81	0	0	2	0
12	B	56	0	0	0	0
12	C	83	0	0	1	0
12	D	33	0	0	1	0
12	H	42	0	0	0	0
12	J	21	0	0	0	0
12	K	55	0	0	2	0
12	L	46	0	0	0	0
All	All	21069	0	20136	171	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 4.

The worst 5 of 171 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:C:393:LYS:HD2	1:C:394:ASN:H	1.15	1.04
2:D:257:GLN:HE21	2:D:261:ASN:H	1.06	0.94
2:D:257:GLN:HA	2:D:259:ILE:H	1.30	0.94
2:D:257:GLN:NE2	2:D:261:ASN:H	1.75	0.84
2:B:92:LEU:O	2:B:398:HIS:ND1	2.12	0.81

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	421/461 (91%)	400 (95%)	20 (5%)	1 (0%)	47	71
1	C	425/461 (92%)	409 (96%)	14 (3%)	2 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	447/478 (94%)	434 (97%)	12 (3%)	1 (0%)	47	71
2	D	402/478 (84%)	376 (94%)	23 (6%)	3 (1%)	22	43
3	H	215/225 (96%)	208 (97%)	7 (3%)	0	100	100
3	J	214/225 (95%)	205 (96%)	6 (3%)	3 (1%)	11	22
4	K	214/217 (99%)	207 (97%)	6 (3%)	1 (0%)	29	52
4	L	215/217 (99%)	206 (96%)	8 (4%)	1 (0%)	29	52
All	All	2553/2762 (92%)	2445 (96%)	96 (4%)	12 (0%)	29	52

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	394	ASN
2	D	347	ALA
3	J	137	PRO
3	J	201	SER
1	A	163	GLY

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	380/407 (93%)	377 (99%)	3 (1%)	81	92
1	C	383/407 (94%)	381 (100%)	2 (0%)	88	96
2	B	405/428 (95%)	401 (99%)	4 (1%)	76	90
2	D	362/428 (85%)	354 (98%)	8 (2%)	52	76
3	H	189/192 (98%)	188 (100%)	1 (0%)	88	96
3	J	187/192 (97%)	183 (98%)	4 (2%)	53	77
4	K	190/191 (100%)	187 (98%)	3 (2%)	62	82
4	L	191/191 (100%)	189 (99%)	2 (1%)	76	90
All	All	2287/2436 (94%)	2260 (99%)	27 (1%)	71	87

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	257	GLN
2	D	376	GLU
4	K	131	SER
2	D	315	ASP
2	B	265	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	155	ASN
1	C	304	GLN
2	D	257	GLN
2	B	243	GLN
2	D	49	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 ⓘ

5 monosaccharides 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	$\# Z > 2$
5	NAG	E	1	2,5	14,14,15	0.59	0	17,19,21	0.93	0
5	NAG	E	2	5	14,14,15	0.59	0	17,19,21	1.71	5 (29%)
5	BMA	E	3	5	11,11,12	0.64	0	15,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	F	1	2,6	14,14,15	0.55	0	17,19,21	1.00	1 (5%)
6	NAG	F	2	6	14,14,15	0.40	0	17,19,21	1.50	2 (11%)

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
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	2	NAG	C1-O5-C5	4.23	117.92	112.19
5	E	2	NAG	C1-O5-C5	3.25	116.60	112.19
5	E	2	NAG	C3-C4-C5	3.02	115.62	110.24
6	F	1	NAG	C1-O5-C5	2.89	116.10	112.19
5	E	2	NAG	C2-N2-C7	-2.82	118.89	122.90

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
6	F	2	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 5 are monoatomic - leaving 27 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	$\# Z > 2$
7	NAG	B	907	2	14,14,15	0.46	0	17,19,21	0.91	1 (5%)
7	NAG	A	902	1	14,14,15	0.59	0	17,19,21	0.83	0
7	NAG	B	906	2	14,14,15	0.37	0	17,19,21	2.05	3 (17%)
7	NAG	A	903	1	14,14,15	0.54	0	17,19,21	1.15	1 (5%)
7	NAG	C	905	1	14,14,15	0.95	1 (7%)	17,19,21	1.80	5 (29%)
7	NAG	A	906	1	14,14,15	0.62	0	17,19,21	1.13	2 (11%)
7	NAG	D	905	2	14,14,15	0.52	0	17,19,21	1.58	2 (11%)
7	NAG	C	903	1	14,14,15	0.50	0	17,19,21	1.24	1 (5%)
7	NAG	C	902	1	14,14,15	0.49	0	17,19,21	1.09	2 (11%)
7	NAG	A	901	1	14,14,15	0.66	0	17,19,21	0.95	1 (5%)
7	NAG	C	906	1	14,14,15	0.51	0	17,19,21	1.56	2 (11%)
7	NAG	B	909	2	14,14,15	0.75	1 (7%)	17,19,21	1.70	3 (17%)
7	NAG	C	907	1	14,14,15	0.67	0	17,19,21	1.00	0
7	NAG	C	904	1	14,14,15	0.54	0	17,19,21	1.22	1 (5%)
7	NAG	A	904	1	14,14,15	0.59	0	17,19,21	1.53	3 (17%)
7	NAG	A	905	1	14,14,15	0.50	0	17,19,21	1.46	1 (5%)
7	NAG	C	901	1	14,14,15	0.52	0	17,19,21	0.90	1 (5%)
7	NAG	D	903	2	14,14,15	0.48	0	17,19,21	1.84	2 (11%)
7	NAG	D	904	2	14,14,15	0.45	0	17,19,21	2.04	4 (23%)
7	NAG	B	901	2	14,14,15	0.66	0	17,19,21	1.13	2 (11%)
7	NAG	B	908	2	14,14,15	0.53	0	17,19,21	0.63	0
7	NAG	B	905	2	14,14,15	0.52	0	17,19,21	1.20	2 (11%)
7	NAG	A	907	1	14,14,15	0.53	0	17,19,21	1.22	1 (5%)

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	B	907	2	-	4/6/23/26	0/1/1/1
7	NAG	A	902	1	-	3/6/23/26	0/1/1/1
7	NAG	B	906	2	-	4/6/23/26	0/1/1/1
7	NAG	A	903	1	-	4/6/23/26	0/1/1/1
7	NAG	C	905	1	-	2/6/23/26	0/1/1/1
7	NAG	A	906	1	-	2/6/23/26	0/1/1/1
7	NAG	D	905	2	-	4/6/23/26	0/1/1/1
7	NAG	C	903	1	-	2/6/23/26	0/1/1/1
7	NAG	C	902	1	-	3/6/23/26	0/1/1/1
7	NAG	A	901	1	-	2/6/23/26	0/1/1/1
7	NAG	C	906	1	-	2/6/23/26	0/1/1/1
7	NAG	B	909	2	-	4/6/23/26	0/1/1/1
7	NAG	C	907	1	-	2/6/23/26	0/1/1/1
7	NAG	C	904	1	-	2/6/23/26	0/1/1/1
7	NAG	A	904	1	-	2/6/23/26	0/1/1/1
7	NAG	A	905	1	-	3/6/23/26	0/1/1/1
7	NAG	C	901	1	-	2/6/23/26	0/1/1/1
7	NAG	D	903	2	-	2/6/23/26	0/1/1/1
7	NAG	D	904	2	-	2/6/23/26	0/1/1/1
7	NAG	B	901	2	-	2/6/23/26	0/1/1/1
7	NAG	B	908	2	-	2/6/23/26	0/1/1/1
7	NAG	B	905	2	-	4/6/23/26	0/1/1/1
7	NAG	A	907	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	909	NAG	O5-C1	-2.19	1.40	1.43
7	C	905	NAG	C2-N2	-2.06	1.42	1.46

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	D	904	NAG	C1-O5-C5	6.59	121.12	112.19
7	D	903	NAG	C1-O5-C5	6.15	120.53	112.19
7	B	906	NAG	C1-O5-C5	5.84	120.11	112.19
7	C	906	NAG	C1-O5-C5	4.70	118.56	112.19
7	A	905	NAG	C1-O5-C5	4.53	118.33	112.19

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	905	NAG	O5-C5-C6-O6
7	B	907	NAG	O5-C5-C6-O6
7	B	905	NAG	C4-C5-C6-O6
7	D	905	NAG	O5-C5-C6-O6
7	B	906	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	902	NAG	1	0
7	B	906	NAG	1	0
7	A	901	NAG	1	0
7	C	904	NAG	1	0
7	C	901	NAG	1	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 ⓘ

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	427/461 (92%)	-0.40	3 (0%) 87 86	20, 35, 64, 80	0
1	C	430/461 (93%)	-0.43	4 (0%) 84 82	19, 35, 65, 83	0
2	B	453/478 (94%)	-0.44	1 (0%) 95 95	22, 43, 72, 89	0
2	D	414/478 (86%)	-0.03	19 (4%) 32 26	25, 58, 107, 137	0
3	H	219/225 (97%)	-0.36	0 100 100	18, 39, 69, 85	0
3	J	218/225 (96%)	-0.34	1 (0%) 91 89	22, 42, 71, 82	0
4	K	216/217 (99%)	-0.49	0 100 100	19, 34, 56, 73	0
4	L	217/217 (100%)	-0.56	0 100 100	17, 33, 57, 74	0
All	All	2594/2762 (93%)	-0.36	28 (1%) 80 78	17, 39, 76, 137	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	291	ASN	4.3
2	D	260	ILE	4.2
2	D	474	ILE	4.2
2	D	208	ASN	3.8
2	D	319	THR	3.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. 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	B-factors(Å ²)	Q<0.9
5	BMA	E	3	11/12	0.76	0.20	68,84,93,96	0
6	NAG	F	2	14/15	0.82	0.32	62,73,84,93	0
5	NAG	E	2	14/15	0.90	0.17	44,64,72,75	0
6	NAG	F	1	14/15	0.93	0.13	44,52,59,64	0
5	NAG	E	1	14/15	0.97	0.12	39,54,62,63	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. 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	B-factors(Å ²)	Q<0.9
7	NAG	C	902	14/15	0.73	0.43	70,76,86,97	0
7	NAG	B	906	14/15	0.78	0.26	99,109,111,116	0
7	NAG	A	903	14/15	0.78	0.24	62,78,84,89	0
7	NAG	B	907	14/15	0.78	0.37	83,92,98,98	0
7	NAG	D	905	14/15	0.80	0.44	81,91,98,101	0
7	NAG	B	908	14/15	0.80	0.45	59,85,97,98	0
7	NAG	A	902	14/15	0.81	0.37	74,81,86,92	0
7	NAG	A	907	14/15	0.82	0.25	68,83,87,94	0
7	NAG	B	901	14/15	0.83	0.34	82,95,106,109	0
11	CA	K	301	1/1	0.89	0.40	86,86,86,86	0
7	NAG	C	903	14/15	0.89	0.30	60,69,82,87	0
7	NAG	A	905	14/15	0.90	0.15	53,68,77,79	0
7	NAG	D	904	14/15	0.90	0.31	92,101,121,127	0
8	GLU	D	951	10/10	0.91	0.30	52,61,88,96	0
7	NAG	B	909	14/15	0.91	0.32	68,75,84,91	0
7	NAG	C	905	14/15	0.92	0.19	40,57,71,72	0
7	NAG	C	904	14/15	0.92	0.24	55,63,76,80	0
7	NAG	B	905	14/15	0.93	0.19	66,75,92,92	0
7	NAG	A	906	14/15	0.94	0.12	42,53,61,68	0
7	NAG	D	903	14/15	0.94	0.20	46,55,74,87	0
9	NA	A	961	1/1	0.95	0.07	39,39,39,39	0
7	NAG	C	907	14/15	0.95	0.14	41,52,63,72	0
10	CL	D	971	1/1	0.95	0.51	107,107,107,107	0
7	NAG	A	904	14/15	0.95	0.19	48,55,77,78	0
7	NAG	C	901	14/15	0.96	0.13	29,36,48,49	0
7	NAG	A	901	14/15	0.96	0.12	33,37,46,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	C	906	14/15	0.96	0.12	40,48,55,57	0
8	GLU	C	951	10/10	0.96	0.17	42,46,70,84	0
8	GLU	B	951	10/10	0.97	0.15	25,44,64,67	0
8	GLU	A	951	10/10	0.97	0.16	25,34,61,65	0
9	NA	C	961	1/1	0.98	0.09	26,26,26,26	0
10	CL	B	971	1/1	0.98	0.52	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.