



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:10 PM GMT

PDB ID : 5F9T  
Title : Crystal Structure of Streptococcus pneumoniae NanC, covalent complex with a fluorinated Neu5Ac derivative  
Authors : Owen, C.D.; Lukacik, P.; Potter, J.A.; Walsh, M.; Taylor, G.L.  
Deposited on : 2015-12-10  
Resolution : 2.05 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

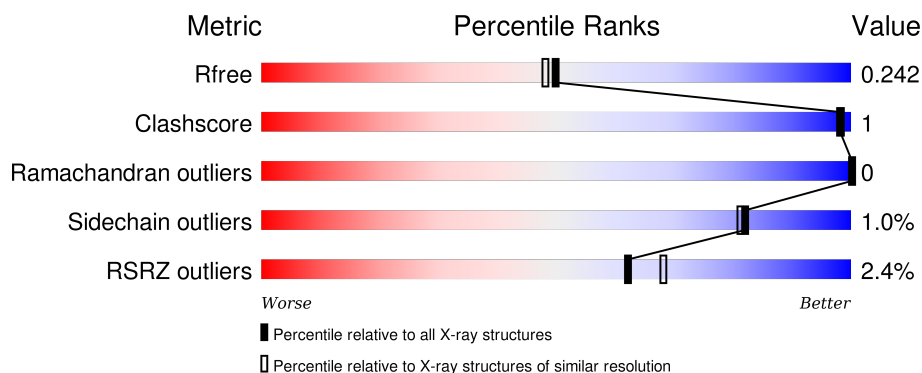
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	659	 2% 96% . .
1	B	659	 3% 97% .

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
3	SFJ	B	803	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11106 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.

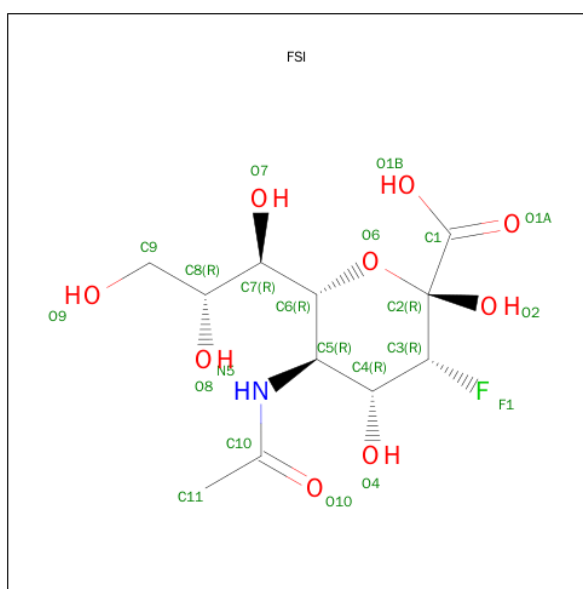
- Molecule 1 is a protein called Neuraminidase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	1	0
			5230	3321	881	1017	11			
1	B	659	Total	C	N	O	S	0	1	0
			5231	3321	881	1019	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	LEU	-	expression tag	UNP A0A0I8L4I1
B	741	LEU	-	expression tag	UNP A0A0I8L4I1

- Molecule 2 is 5-(acetylamino)-3,5-dideoxy-3-fluoro-D-erythro- $\alpha$ -L-manno-non-2-ulopyranosonic acid (three-letter code: FSI) (formula: C<sub>11</sub>H<sub>18</sub>FNO<sub>9</sub>).



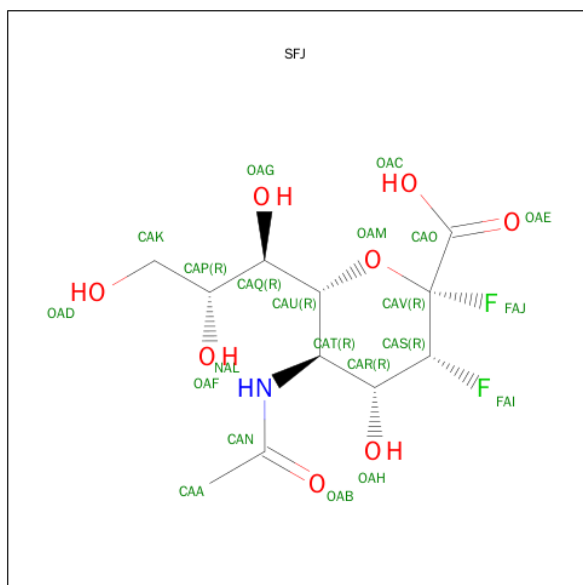
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			21	11	1	1	8		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			21	11	1	1	8		

- Molecule 3 is (2R,3R,4R,5R,6R)-5-(acetylamino)-2,3-difluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]tetrahydro-2H-pyran-2-carboxylic acid (three-letter code: SFJ) (formula: C<sub>11</sub>H<sub>17</sub>F<sub>2</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	11	2	1	8		
3	B	1	Total	C	F	N	O	0	0
			22	11	2	1	8		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

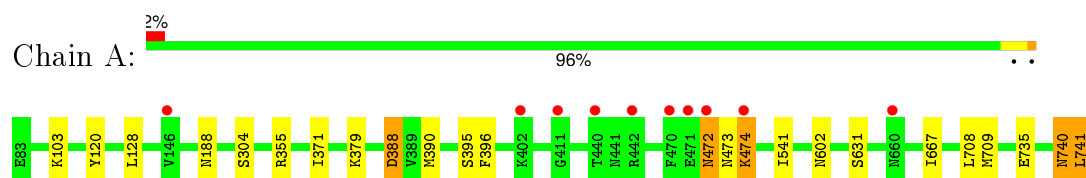
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	322	Total	O	0	0
			322	322		
5	B	231	Total	O	0	0
			231	231		

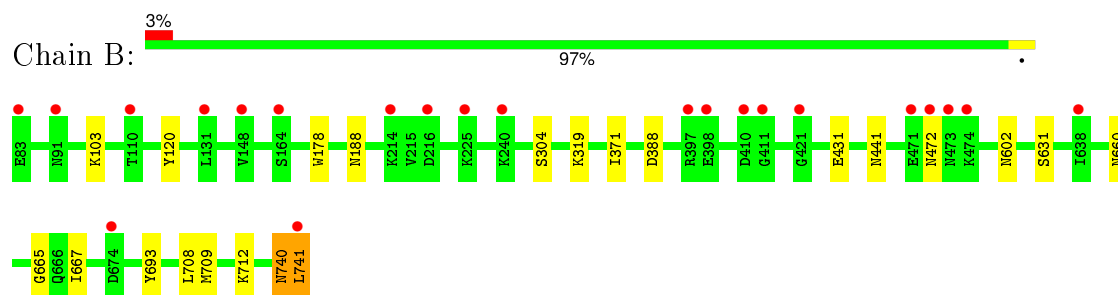
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Neuraminidase C



#### • Molecule 1: Neuraminidase C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.24Å 74.84Å 113.35Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 23.63 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.05) 97.5 (23.63-2.05)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.198 , 0.235 0.206 , 0.242	Depositor DCC
$R_{free}$ test set	5104 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 101995 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SFJ, FSI

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	0.53	0/5350	0.72	2/7252 (0.0%)
1	B	0.52	0/5351	0.72	0/7253
All	All	0.53	0/10701	0.72	2/14505 (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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	388	ASP	CB-CG-OD1	5.36	123.12	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	740	ASN	Peptide
1	B	740	ASN	Peptide

## 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	5230	0	5116	12	0
1	B	5231	0	5112	9	0
2	A	21	0	16	0	0
2	B	21	0	16	0	0
3	A	22	0	16	1	0
3	B	22	0	16	0	0
4	B	6	0	8	0	0
5	A	322	0	0	0	0
5	B	231	0	0	0	0
All	All	11106	0	10300	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 1.

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:B:431[B]:GLU:HG2	1:B:431[B]:GLU:O	1.86	0.74
1:A:474:LYS:HE3	1:A:474:LYS:HA	1.89	0.53
1:A:304:SER:HB2	1:A:709:MET:HE1	1.93	0.50
1:B:667:ILE:HD11	1:B:708:LEU:HD22	1.93	0.50
1:A:740:ASN:O	1:A:741:LEU:HB2	2.12	0.49
1:A:396:PHE:CD1	1:A:396:PHE:N	2.80	0.49
1:B:740:ASN:O	1:B:741:LEU:HB2	2.14	0.48
1:B:304:SER:HB2	1:B:709:MET:HE1	1.95	0.48
1:A:667:ILE:HD11	1:A:708:LEU:HD22	1.95	0.48
1:A:602:ASN:HA	1:A:631:SER:O	2.14	0.48
1:A:128:LEU:HD21	3:A:802:SFJ:H2	1.96	0.47
1:B:602:ASN:HA	1:B:631:SER:O	2.13	0.47
1:B:371:ILE:HG23	1:B:388:ASP:HB2	2.00	0.44
1:B:178:TRP:CD1	1:B:712:LYS:HE2	2.55	0.42
1:A:472:ASN:HA	1:A:473:ASN:HA	1.92	0.42
1:A:371:ILE:HG23	1:A:388:ASP:HB2	2.02	0.42
1:B:665:GLY:HA3	1:B:693:TYR:CG	2.54	0.41
1:B:120:TYR:CE1	1:B:188:ASN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:HE2	1:A:541:ILE:HG21	2.03	0.41
1:A:390[A]:MET:HG3	1:A:396:PHE:CE1	2.56	0.41
1:A:120:TYR:CE1	1:A:188:ASN:HB2	2.56	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	658/659 (100%)	640 (97%)	18 (3%)	0	100	100
1	B	658/659 (100%)	642 (98%)	16 (2%)	0	100	100
All	All	1316/1318 (100%)	1282 (97%)	34 (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	574/573 (100%)	568 (99%)	6 (1%)	82	81
1	B	574/573 (100%)	568 (99%)	6 (1%)	82	81
All	All	1148/1146 (100%)	1136 (99%)	12 (1%)	82	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	395	SER
1	A	472	ASN
1	A	474	LYS
1	A	735	GLU
1	A	741	LEU
1	B	103	LYS
1	B	319	LYS
1	B	441	ASN
1	B	472	ASN
1	B	660	ASN
1	B	741	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	183	GLN
1	A	246	ASN
1	A	459	ASN
1	B	246	ASN
1	B	441	ASN
1	B	472	ASN
1	B	511	HIS
1	B	676	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 ⓘ

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	$\# Z  > 2$
2	FSI	A	801	1	18,21,22	0.87	1 (5%)	21,30,33	1.06	1 (4%)
3	SFJ	A	802	-	16,22,22	0.46	0	19,33,33	0.72	0
4	GOL	B	801	-	5,5,5	0.24	0	5,5,5	0.41	0
2	FSI	B	802	1	18,21,22	0.67	0	21,30,33	0.97	1 (4%)
3	SFJ	B	803	-	16,22,22	0.44	0	19,33,33	0.84	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
2	FSI	A	801	1	-	0/14/38/43	0/1/1/1
3	SFJ	A	802	-	-	0/14/43/43	0/1/1/1
4	GOL	B	801	-	-	0/4/4/4	0/0/0/0
2	FSI	B	802	1	-	0/14/38/43	0/1/1/1
3	SFJ	B	803	-	-	0/14/43/43	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FSI	C3-C2	3.06	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	FSI	C7-C6-C5	-2.06	111.22	114.06
2	A	801	FSI	F1-C3-C2	3.11	111.96	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	SFJ	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	659/659 (100%)	-0.19	10 (1%) 76 81	16, 27, 51, 116	0
1	B	659/659 (100%)	0.03	22 (3%) 50 57	18, 34, 58, 87	0
All	All	1318/1318 (100%)	-0.08	32 (2%) 62 68	16, 31, 56, 116	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	ASN	6.3
1	A	471	GLU	5.7
1	A	442	ARG	4.5
1	B	741	LEU	4.0
1	B	472	ASN	4.0
1	B	164	SER	3.2
1	B	474	LYS	3.2
1	B	398	GLU	3.0
1	B	148	VAL	2.9
1	B	471	GLU	2.7
1	B	674	ASP	2.6
1	B	131	LEU	2.5
1	B	240	LYS	2.4
1	B	216	ASP	2.4
1	A	660	ASN	2.3
1	B	410	ASP	2.3
1	B	397	ARG	2.3
1	A	470	PHE	2.2
1	A	146	VAL	2.2
1	B	421	GLY	2.2
1	B	473	ASN	2.2
1	B	411	GLY	2.1
1	B	110	THR	2.1
1	B	225	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	91	ASN	2.1
1	B	638	ILE	2.1
1	A	474	LYS	2.1
1	A	440	THR	2.1
1	B	83	GLU	2.0
1	A	402	LYS	2.0
1	B	214	LYS	2.0
1	A	411	GLY	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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	SFJ	B	803	22/22	0.92	0.18	2.40	26,37,54,64	0
4	GOL	B	801	6/6	0.92	0.13	1.31	33,36,43,52	0
3	SFJ	A	802	22/22	0.91	0.13	1.24	22,31,39,53	0
2	FSI	A	801	21/22	0.95	0.10	-0.42	15,20,32,59	0
2	FSI	B	802	21/22	0.96	0.09	-0.85	15,23,37,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.