Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 02:25 PM EDT

PDB ID	:	6XSW
Title	:	Structure of the Notch3 NRR in complex with an antibody Fab Fragment
Authors	:	Bard, J.
Deposited on	:	2020-07-16
Resolution	:	2.98 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

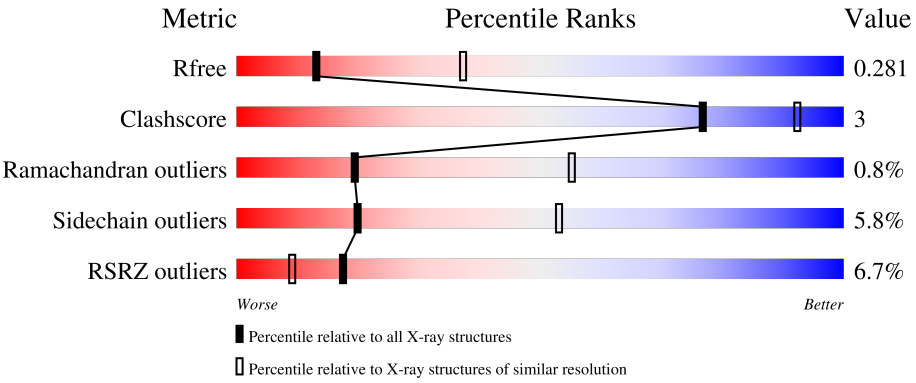
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 of 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 <=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	231	2% 83% 10% 7%
1	D	231	11% 69% 10% 20%
1	G	231	10% 81% 12% 7%
1	H	231	2% 82% 12% 6%
2	B	214	5% 84% 14%

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Mol	Chain	Length	Quality of chain
2	E	214	6% 60% 7% 33%
2	I	214	17% 86% 13%
2	L	214	89% 11%
3	C	280	3% 71% 7% 21%
3	F	280	4% 74% 8% 18%
3	J	280	9% 69% 9% 22%
3	X	280	% 69% 13% 18%
4	P	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18917 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 Anti-N3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1611	1022	269	314	6			
1	D	184	Total	C	N	O	S	0	0	0
			1371	871	229	265	6			
1	G	215	Total	C	N	O	S	0	0	0
			1591	1011	263	311	6			
1	H	217	Total	C	N	O	S	0	0	0
			1629	1036	271	316	6			

- Molecule 2 is a protein called Anti-N3 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1621	1016	273	327	5			
2	E	144	Total	C	N	O	S	0	0	0
			1070	670	176	221	3			
2	I	211	Total	C	N	O	S	0	0	0
			1594	1001	265	323	5			
2	L	213	Total	C	N	O	S	0	0	0
			1639	1028	275	331	5			

- Molecule 3 is a protein called Neurogenic locus notch homolog protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1648	1021	290	316	21			
3	F	229	Total	C	N	O	S	0	0	0
			1714	1057	301	335	21			
3	J	218	Total	C	N	O	S	0	0	0
			1613	994	282	316	21			
3	X	231	Total	C	N	O	S	0	0	0
			1737	1071	312	332	22			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1342	MET	-	expression tag	UNP Q9UM47
C	1343	GLU	-	expression tag	UNP Q9UM47
C	1344	THR	-	expression tag	UNP Q9UM47
C	1345	ASP	-	expression tag	UNP Q9UM47
C	1346	THR	-	expression tag	UNP Q9UM47
C	1347	LEU	-	expression tag	UNP Q9UM47
C	1348	LEU	-	expression tag	UNP Q9UM47
C	1349	LEU	-	expression tag	UNP Q9UM47
C	1350	TRP	-	expression tag	UNP Q9UM47
C	1351	VAL	-	expression tag	UNP Q9UM47
C	1352	LEU	-	expression tag	UNP Q9UM47
C	1353	LEU	-	expression tag	UNP Q9UM47
C	1354	LEU	-	expression tag	UNP Q9UM47
C	1355	TRP	-	expression tag	UNP Q9UM47
C	1356	VAL	-	expression tag	UNP Q9UM47
C	1357	PRO	-	expression tag	UNP Q9UM47
C	1358	GLY	-	expression tag	UNP Q9UM47
C	1359	SER	-	expression tag	UNP Q9UM47
C	1360	THR	-	expression tag	UNP Q9UM47
C	1361	GLY	-	expression tag	UNP Q9UM47
C	1362	GLY	-	expression tag	UNP Q9UM47
C	1363	SER	-	expression tag	UNP Q9UM47
C	1364	GLY	-	expression tag	UNP Q9UM47
C	1365	HIS	-	expression tag	UNP Q9UM47
C	1366	HIS	-	expression tag	UNP Q9UM47
C	1367	HIS	-	expression tag	UNP Q9UM47
C	1368	HIS	-	expression tag	UNP Q9UM47
C	1369	HIS	-	expression tag	UNP Q9UM47
C	1370	HIS	-	expression tag	UNP Q9UM47
C	1371	GLY	-	expression tag	UNP Q9UM47
C	1372	GLU	-	expression tag	UNP Q9UM47
C	1373	ASN	-	expression tag	UNP Q9UM47
C	1374	LEU	-	expression tag	UNP Q9UM47
C	1375	TYR	-	expression tag	UNP Q9UM47
C	1376	PHE	-	expression tag	UNP Q9UM47
C	1377	GLN	-	expression tag	UNP Q9UM47
C	1378	SER	-	expression tag	UNP Q9UM47
C	?	-	PRO	deletion	UNP Q9UM47
C	?	-	SER	deletion	UNP Q9UM47
C	?	-	PRO	deletion	UNP Q9UM47
C	?	-	GLY	deletion	UNP Q9UM47
C	?	-	SER	deletion	UNP Q9UM47

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q9UM47
C	?	-	PRO	deletion	UNP Q9UM47
C	?	-	ARG	deletion	UNP Q9UM47
C	?	-	ALA	deletion	UNP Q9UM47
C	?	-	ARG	deletion	UNP Q9UM47
C	?	-	ARG	deletion	UNP Q9UM47
C	?	-	GLU	deletion	UNP Q9UM47
C	?	-	LEU	deletion	UNP Q9UM47
C	?	-	ALA	deletion	UNP Q9UM47
F	1342	MET	-	expression tag	UNP Q9UM47
F	1343	GLU	-	expression tag	UNP Q9UM47
F	1344	THR	-	expression tag	UNP Q9UM47
F	1345	ASP	-	expression tag	UNP Q9UM47
F	1346	THR	-	expression tag	UNP Q9UM47
F	1347	LEU	-	expression tag	UNP Q9UM47
F	1348	LEU	-	expression tag	UNP Q9UM47
F	1349	LEU	-	expression tag	UNP Q9UM47
F	1350	TRP	-	expression tag	UNP Q9UM47
F	1351	VAL	-	expression tag	UNP Q9UM47
F	1352	LEU	-	expression tag	UNP Q9UM47
F	1353	LEU	-	expression tag	UNP Q9UM47
F	1354	LEU	-	expression tag	UNP Q9UM47
F	1355	TRP	-	expression tag	UNP Q9UM47
F	1356	VAL	-	expression tag	UNP Q9UM47
F	1357	PRO	-	expression tag	UNP Q9UM47
F	1358	GLY	-	expression tag	UNP Q9UM47
F	1359	SER	-	expression tag	UNP Q9UM47
F	1360	THR	-	expression tag	UNP Q9UM47
F	1361	GLY	-	expression tag	UNP Q9UM47
F	1362	GLY	-	expression tag	UNP Q9UM47
F	1363	SER	-	expression tag	UNP Q9UM47
F	1364	GLY	-	expression tag	UNP Q9UM47
F	1365	HIS	-	expression tag	UNP Q9UM47
F	1366	HIS	-	expression tag	UNP Q9UM47
F	1367	HIS	-	expression tag	UNP Q9UM47
F	1368	HIS	-	expression tag	UNP Q9UM47
F	1369	HIS	-	expression tag	UNP Q9UM47
F	1370	HIS	-	expression tag	UNP Q9UM47
F	1371	GLY	-	expression tag	UNP Q9UM47
F	1372	GLU	-	expression tag	UNP Q9UM47
F	1373	ASN	-	expression tag	UNP Q9UM47
F	1374	LEU	-	expression tag	UNP Q9UM47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1375	TYR	-	expression tag	UNP Q9UM47
F	1376	PHE	-	expression tag	UNP Q9UM47
F	1377	GLN	-	expression tag	UNP Q9UM47
F	1378	SER	-	expression tag	UNP Q9UM47
F	?	-	PRO	deletion	UNP Q9UM47
F	?	-	SER	deletion	UNP Q9UM47
F	?	-	PRO	deletion	UNP Q9UM47
F	?	-	GLY	deletion	UNP Q9UM47
F	?	-	SER	deletion	UNP Q9UM47
F	?	-	GLU	deletion	UNP Q9UM47
F	?	-	PRO	deletion	UNP Q9UM47
F	?	-	ARG	deletion	UNP Q9UM47
F	?	-	ALA	deletion	UNP Q9UM47
F	?	-	ARG	deletion	UNP Q9UM47
F	?	-	ARG	deletion	UNP Q9UM47
F	?	-	GLU	deletion	UNP Q9UM47
F	?	-	LEU	deletion	UNP Q9UM47
F	?	-	ALA	deletion	UNP Q9UM47
J	1342	MET	-	expression tag	UNP Q9UM47
J	1343	GLU	-	expression tag	UNP Q9UM47
J	1344	THR	-	expression tag	UNP Q9UM47
J	1345	ASP	-	expression tag	UNP Q9UM47
J	1346	THR	-	expression tag	UNP Q9UM47
J	1347	LEU	-	expression tag	UNP Q9UM47
J	1348	LEU	-	expression tag	UNP Q9UM47
J	1349	LEU	-	expression tag	UNP Q9UM47
J	1350	TRP	-	expression tag	UNP Q9UM47
J	1351	VAL	-	expression tag	UNP Q9UM47
J	1352	LEU	-	expression tag	UNP Q9UM47
J	1353	LEU	-	expression tag	UNP Q9UM47
J	1354	LEU	-	expression tag	UNP Q9UM47
J	1355	TRP	-	expression tag	UNP Q9UM47
J	1356	VAL	-	expression tag	UNP Q9UM47
J	1357	PRO	-	expression tag	UNP Q9UM47
J	1358	GLY	-	expression tag	UNP Q9UM47
J	1359	SER	-	expression tag	UNP Q9UM47
J	1360	THR	-	expression tag	UNP Q9UM47
J	1361	GLY	-	expression tag	UNP Q9UM47
J	1362	GLY	-	expression tag	UNP Q9UM47
J	1363	SER	-	expression tag	UNP Q9UM47
J	1364	GLY	-	expression tag	UNP Q9UM47
J	1365	HIS	-	expression tag	UNP Q9UM47

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1366	HIS	-	expression tag	UNP Q9UM47
J	1367	HIS	-	expression tag	UNP Q9UM47
J	1368	HIS	-	expression tag	UNP Q9UM47
J	1369	HIS	-	expression tag	UNP Q9UM47
J	1370	HIS	-	expression tag	UNP Q9UM47
J	1371	GLY	-	expression tag	UNP Q9UM47
J	1372	GLU	-	expression tag	UNP Q9UM47
J	1373	ASN	-	expression tag	UNP Q9UM47
J	1374	LEU	-	expression tag	UNP Q9UM47
J	1375	TYR	-	expression tag	UNP Q9UM47
J	1376	PHE	-	expression tag	UNP Q9UM47
J	1377	GLN	-	expression tag	UNP Q9UM47
J	1378	SER	-	expression tag	UNP Q9UM47
J	?	-	PRO	deletion	UNP Q9UM47
J	?	-	SER	deletion	UNP Q9UM47
J	?	-	PRO	deletion	UNP Q9UM47
J	?	-	GLY	deletion	UNP Q9UM47
J	?	-	SER	deletion	UNP Q9UM47
J	?	-	GLU	deletion	UNP Q9UM47
J	?	-	PRO	deletion	UNP Q9UM47
J	?	-	ARG	deletion	UNP Q9UM47
J	?	-	ALA	deletion	UNP Q9UM47
J	?	-	ARG	deletion	UNP Q9UM47
J	?	-	ARG	deletion	UNP Q9UM47
J	?	-	GLU	deletion	UNP Q9UM47
J	?	-	LEU	deletion	UNP Q9UM47
J	?	-	ALA	deletion	UNP Q9UM47
X	1342	MET	-	expression tag	UNP Q9UM47
X	1343	GLU	-	expression tag	UNP Q9UM47
X	1344	THR	-	expression tag	UNP Q9UM47
X	1345	ASP	-	expression tag	UNP Q9UM47
X	1346	THR	-	expression tag	UNP Q9UM47
X	1347	LEU	-	expression tag	UNP Q9UM47
X	1348	LEU	-	expression tag	UNP Q9UM47
X	1349	LEU	-	expression tag	UNP Q9UM47
X	1350	TRP	-	expression tag	UNP Q9UM47
X	1351	VAL	-	expression tag	UNP Q9UM47
X	1352	LEU	-	expression tag	UNP Q9UM47
X	1353	LEU	-	expression tag	UNP Q9UM47
X	1354	LEU	-	expression tag	UNP Q9UM47
X	1355	TRP	-	expression tag	UNP Q9UM47
X	1356	VAL	-	expression tag	UNP Q9UM47

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Chain	Residue	Modelled	Actual	Comment	Reference
X	1357	PRO	-	expression tag	UNP Q9UM47
X	1358	GLY	-	expression tag	UNP Q9UM47
X	1359	SER	-	expression tag	UNP Q9UM47
X	1360	THR	-	expression tag	UNP Q9UM47
X	1361	GLY	-	expression tag	UNP Q9UM47
X	1362	GLY	-	expression tag	UNP Q9UM47
X	1363	SER	-	expression tag	UNP Q9UM47
X	1364	GLY	-	expression tag	UNP Q9UM47
X	1365	HIS	-	expression tag	UNP Q9UM47
X	1366	HIS	-	expression tag	UNP Q9UM47
X	1367	HIS	-	expression tag	UNP Q9UM47
X	1368	HIS	-	expression tag	UNP Q9UM47
X	1369	HIS	-	expression tag	UNP Q9UM47
X	1370	HIS	-	expression tag	UNP Q9UM47
X	1371	GLY	-	expression tag	UNP Q9UM47
X	1372	GLU	-	expression tag	UNP Q9UM47
X	1373	ASN	-	expression tag	UNP Q9UM47
X	1374	LEU	-	expression tag	UNP Q9UM47
X	1375	TYR	-	expression tag	UNP Q9UM47
X	1376	PHE	-	expression tag	UNP Q9UM47
X	1377	GLN	-	expression tag	UNP Q9UM47
X	1378	SER	-	expression tag	UNP Q9UM47
X	?	-	PRO	deletion	UNP Q9UM47
X	?	-	SER	deletion	UNP Q9UM47
X	?	-	PRO	deletion	UNP Q9UM47
X	?	-	GLY	deletion	UNP Q9UM47
X	?	-	SER	deletion	UNP Q9UM47
X	?	-	GLU	deletion	UNP Q9UM47
X	?	-	PRO	deletion	UNP Q9UM47
X	?	-	ARG	deletion	UNP Q9UM47
X	?	-	ALA	deletion	UNP Q9UM47
X	?	-	ARG	deletion	UNP Q9UM47
X	?	-	ARG	deletion	UNP Q9UM47
X	?	-	GLU	deletion	UNP Q9UM47
X	?	-	LEU	deletion	UNP Q9UM47
X	?	-	ALA	deletion	UNP Q9UM47

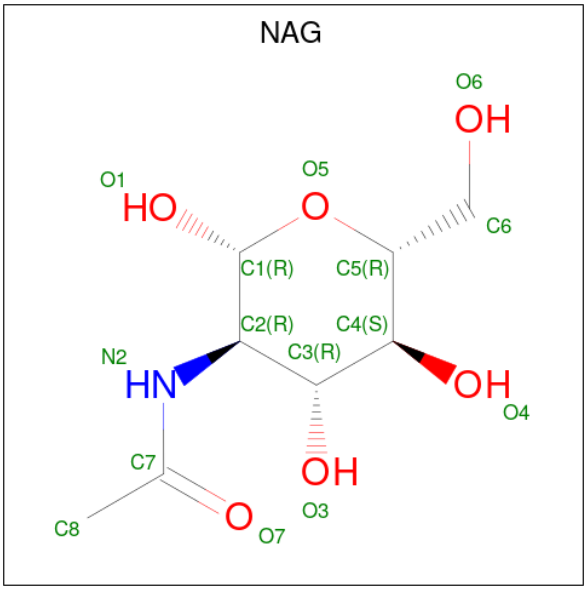
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	3	Total Ca 3 3	0	0
5	F	3	Total Ca 3 3	0	0
5	J	3	Total Ca 3 3	0	0
5	X	4	Total Ca 4 4	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

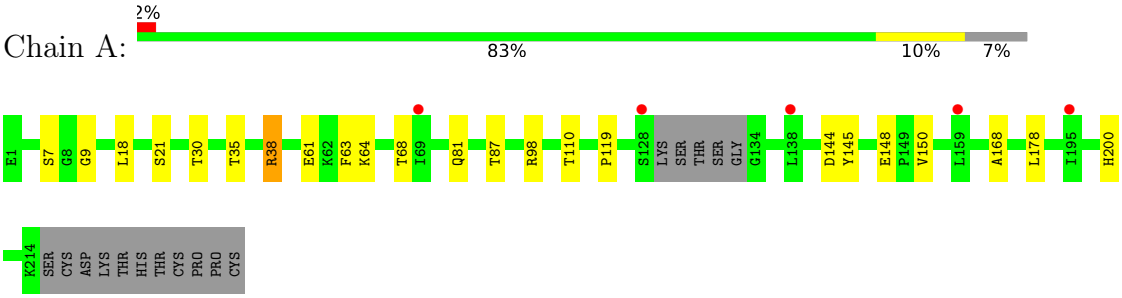
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total O 5 5	0	0
7	G	1	Total O 1 1	0	0
7	H	2	Total O 2 2	0	0
7	J	1	Total O 1 1	0	0
7	L	1	Total O 1 1	0	0

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.

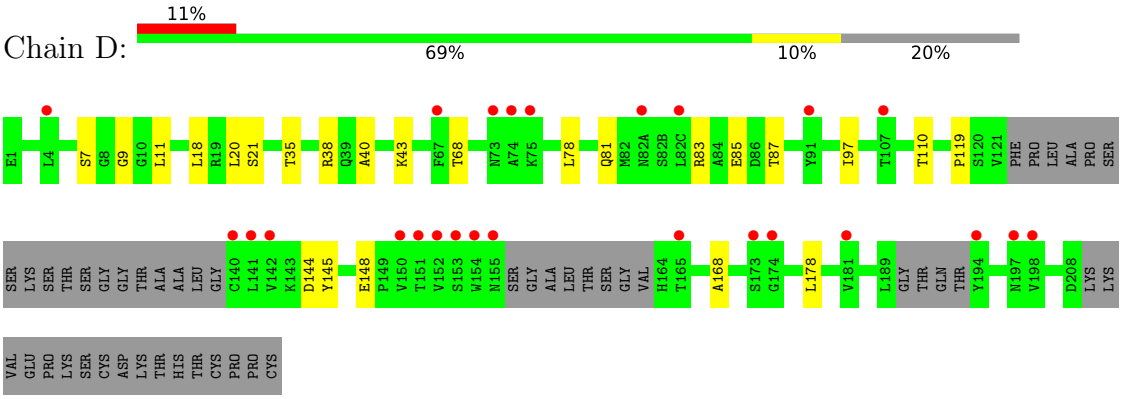
• Molecule 1: Anti-N3 Fab Heavy Chain

Chain A:



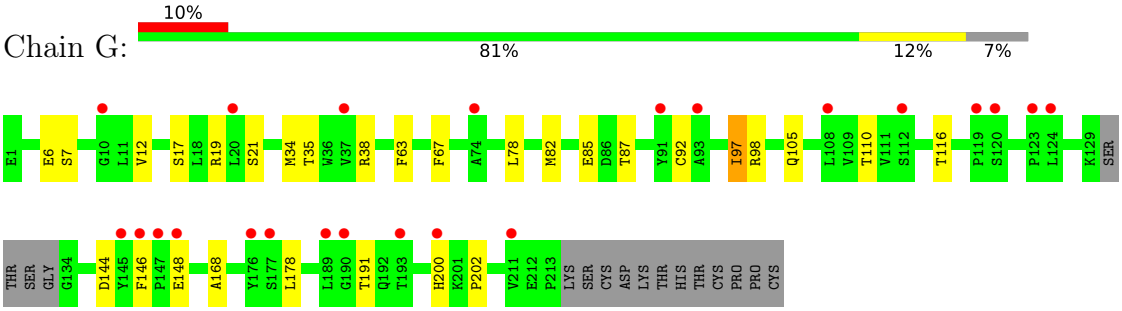
• Molecule 1: Anti-N3 Fab Heavy Chain

Chain D:



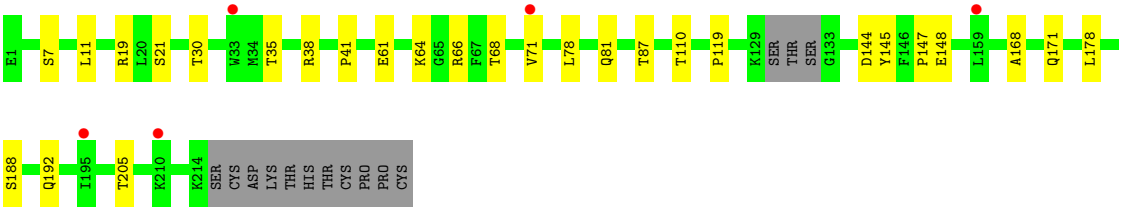
• Molecule 1: Anti-N3 Fab Heavy Chain

Chain G:

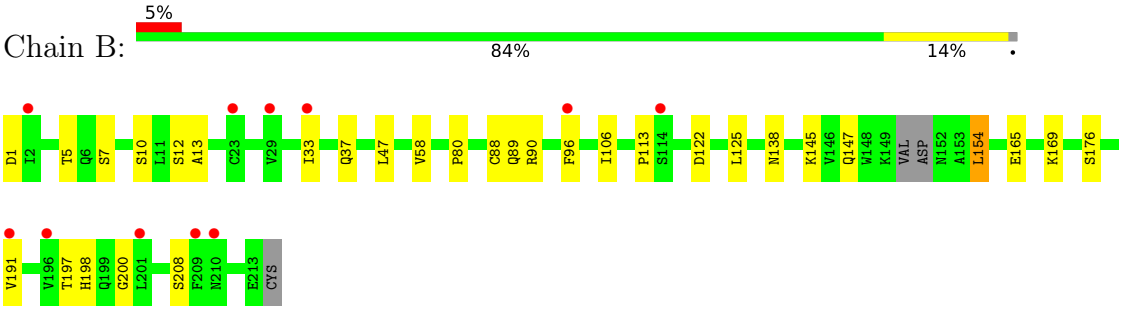


• Molecule 1: Anti-N3 Fab Heavy Chain

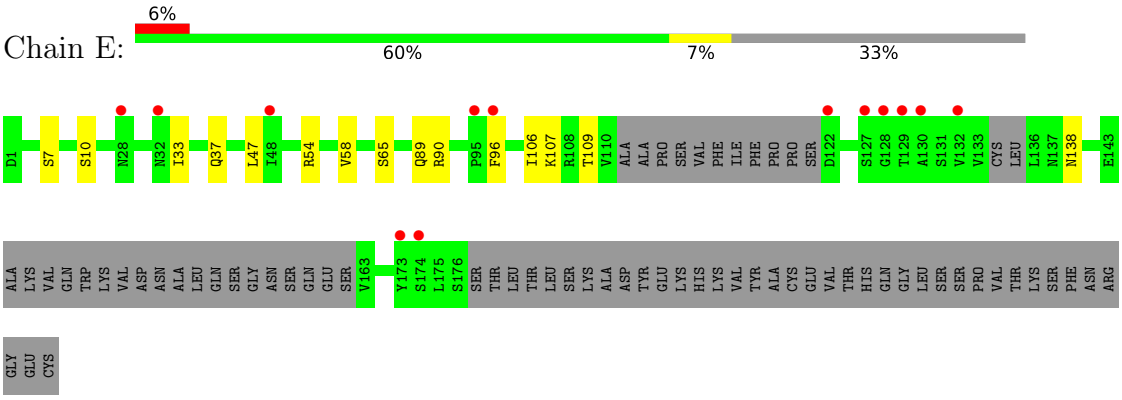
Chain H:



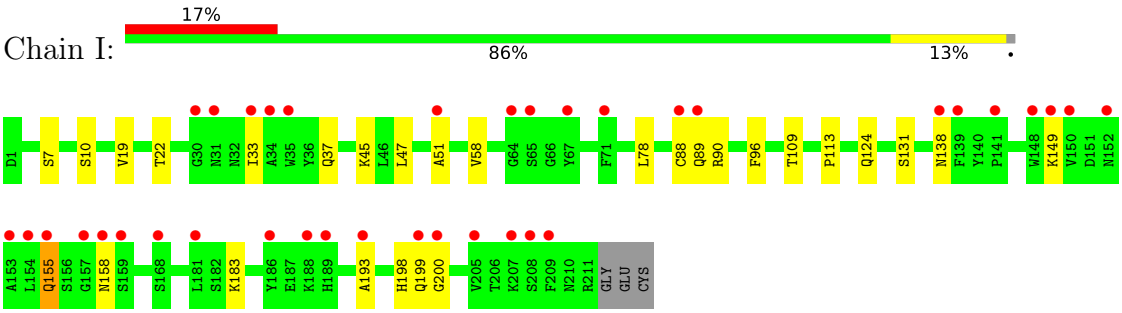
• Molecule 2: Anti-N3 Fab Light Chain



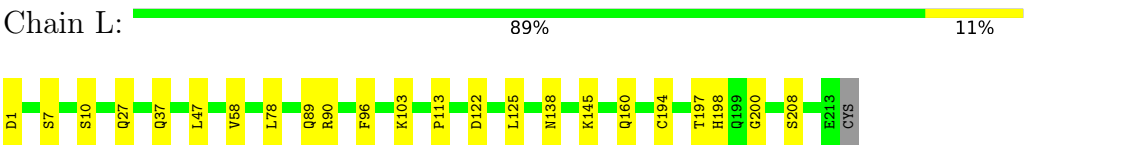
• Molecule 2: Anti-N3 Fab Light Chain



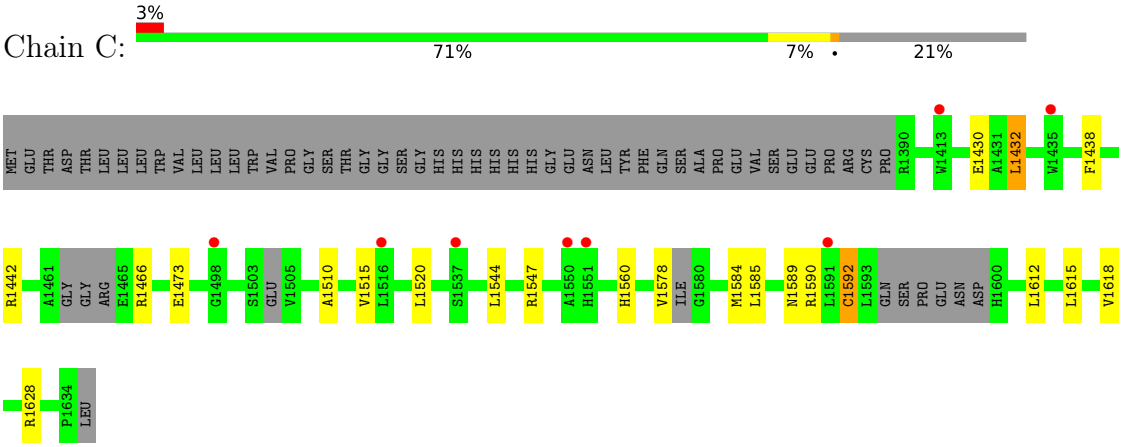
• Molecule 2: Anti-N3 Fab Light Chain



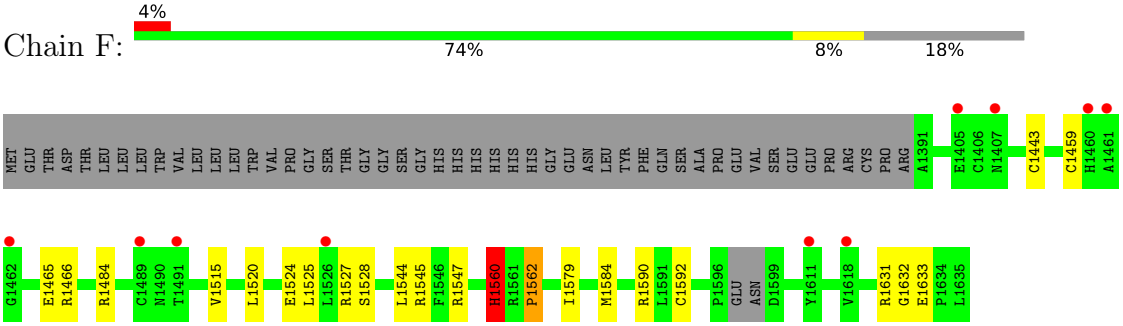
• Molecule 2: Anti-N3 Fab Light Chain



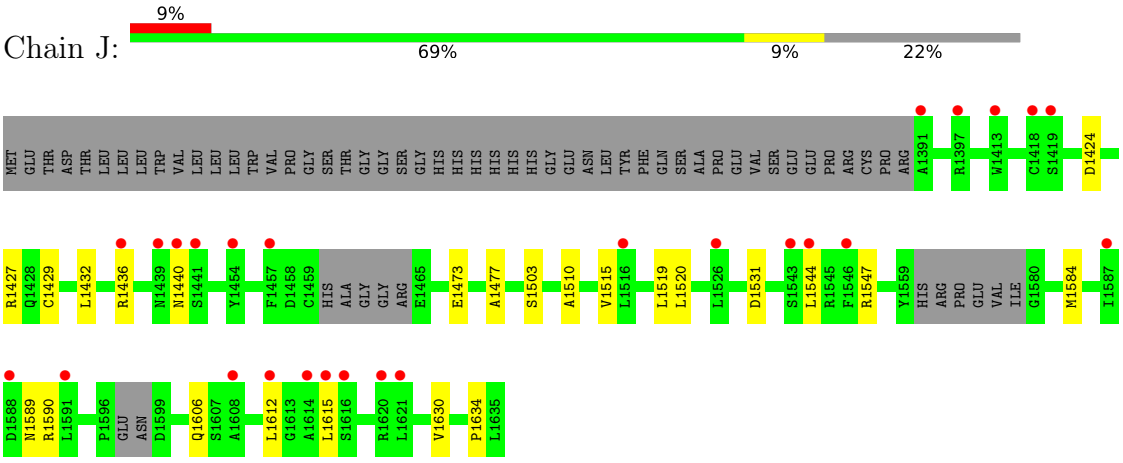
• Molecule 3: Neurogenic locus notch homolog protein 3



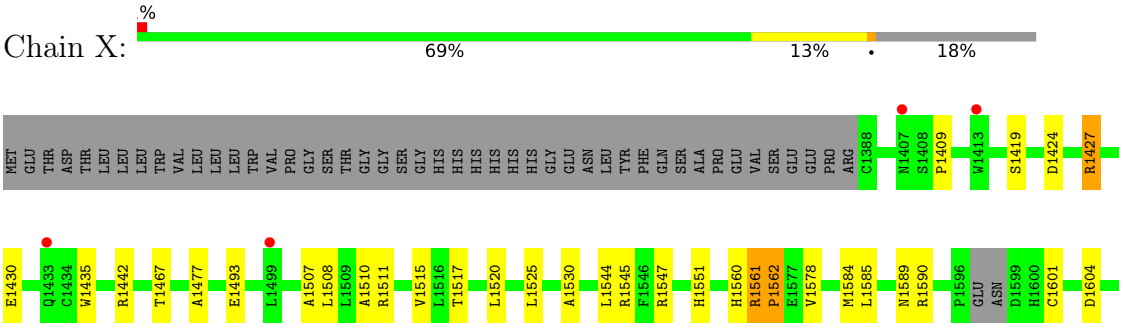
• Molecule 3: Neurogenic locus notch homolog protein 3



• Molecule 3: Neurogenic locus notch homolog protein 3

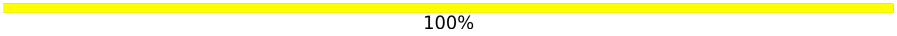


• Molecule 3: Neurogenic locus notch homolog protein 3



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

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.65Å 158.95Å 159.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.66 – 2.98 112.65 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.66-2.98) 99.9 (112.65-2.98)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.233 , 0.256 0.252 , 0.281	Depositor DCC
R_{free} test set	3541 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	57.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	18917	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, NAG

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	0.36	0/1653	0.64	0/2257
1	D	0.37	0/1407	0.64	0/1920
1	G	0.39	0/1633	0.66	0/2236
1	H	0.36	0/1671	0.67	1/2278 (0.0%)
2	B	0.37	0/1657	0.61	0/2250
2	E	0.37	0/1091	0.62	0/1483
2	I	0.38	0/1631	0.61	0/2224
2	L	0.36	0/1676	0.61	0/2278
3	C	0.41	0/1683	0.64	0/2288
3	F	0.41	0/1754	0.66	0/2390
3	J	0.42	0/1647	0.67	0/2244
3	X	0.43	0/1778	0.65	0/2420
All	All	0.39	0/19281	0.64	1/26268 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	41	PRO	C-N-CA	6.62	136.20	122.30

There are no chirality outliers.

There are no planarity outliers.

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	1611	0	1540	10	0
1	D	1371	0	1243	8	0
1	G	1591	0	1498	13	0
1	H	1629	0	1576	10	0
2	B	1621	0	1553	12	0
2	E	1070	0	969	3	0
2	I	1594	0	1500	12	0
2	L	1639	0	1576	9	0
3	C	1648	0	1496	6	0
3	F	1714	0	1543	8	0
3	J	1613	0	1439	7	0
3	X	1737	0	1581	15	0
4	P	28	0	25	0	0
5	C	3	0	0	0	0
5	F	3	0	0	0	0
5	J	3	0	0	0	0
5	X	4	0	0	0	0
6	C	14	0	13	0	0
6	F	14	0	13	0	0
7	A	5	0	0	0	0
7	G	1	0	0	0	0
7	H	2	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
All	All	18917	0	17565	108	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 3.

All (108) 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:G:97:ILE:HG21	3:J:1519:LEU:HD13	1.36	1.08
3:X:1561:ARG:HG2	3:X:1562:PRO:HD3	1.56	0.86
3:J:1477:ALA:HB1	3:J:1531:ASP:HB3	1.63	0.81
2:I:155:GLN:HG2	2:I:158:ASN:HD21	1.49	0.77
1:G:97:ILE:HG21	3:J:1519:LEU:CD1	2.18	0.72
2:B:89:GLN:HE21	2:B:96:PHE:HB3	1.54	0.71
3:F:1443:CYS:HG	3:F:1459:CYS:HG	1.35	0.71
2:E:89:GLN:HE21	2:E:96:PHE:HB3	1.56	0.70
3:X:1561:ARG:HG2	3:X:1562:PRO:CD	2.26	0.63
2:I:89:GLN:HE21	2:I:96:PHE:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1432:LEU:HD11	3:F:1562:PRO:HD3	1.81	0.62
1:G:97:ILE:HG23	1:G:98:ARG:N	2.19	0.57
1:D:9:GLY:HA2	1:D:18:LEU:HD21	1.85	0.57
3:X:1517:THR:HB	3:X:1629:ASP:H	1.69	0.57
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.86	0.57
1:G:34:MET:HB3	1:G:78:LEU:HD22	1.85	0.57
2:I:37:GLN:HB2	2:I:47:LEU:HD11	1.88	0.54
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.88	0.54
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.90	0.54
2:B:33:ILE:HD11	2:B:88:CYS:HB2	1.89	0.54
3:F:1560:HIS:HD2	3:F:1579:ILE:HG12	1.72	0.53
3:X:1424:ASP:HB3	3:X:1427:ARG:HG2	1.90	0.53
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.90	0.53
1:D:87:THR:HG23	1:D:110:THR:HA	1.90	0.53
3:X:1409:PRO:HG3	3:X:1435:TRP:CE2	2.45	0.52
3:X:1419:SER:HB3	3:X:1617:ALA:HB2	1.93	0.51
1:A:150:VAL:HG12	1:A:200:HIS:HB2	1.94	0.50
3:F:1631:ARG:HD3	3:F:1633:GLU:HB2	1.94	0.50
2:B:5:THR:HG23	2:I:199:GLN:HE22	1.77	0.49
2:B:80:PRO:HA	2:B:106:ILE:HD13	1.94	0.49
2:L:198:HIS:CD2	2:L:200:GLY:H	2.31	0.49
2:B:198:HIS:CD2	2:B:200:GLY:H	2.31	0.49
1:A:38:ARG:NH2	1:A:63:PHE:HE1	2.11	0.48
2:I:198:HIS:CD2	2:I:200:GLY:H	2.31	0.48
3:X:1561:ARG:CG	3:X:1562:PRO:HD3	2.35	0.48
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.95	0.48
2:I:33:ILE:HG23	2:I:51:ALA:HA	1.96	0.48
3:X:1511:ARG:HG2	3:X:1604:ASP:HB3	1.96	0.47
1:A:9:GLY:HA2	1:A:18:LEU:HD21	1.97	0.47
3:X:1477:ALA:O	3:X:1530:ALA:HB1	2.15	0.47
3:C:1612:LEU:HA	3:C:1615:LEU:HD12	1.96	0.47
2:L:122:ASP:HA	2:L:125:LEU:HD12	1.95	0.47
2:L:145:LYS:HB3	2:L:197:THR:HB	1.97	0.47
3:J:1424:ASP:O	3:J:1427:ARG:HB2	2.15	0.47
2:B:145:LYS:HB3	2:B:197:THR:HB	1.97	0.47
1:G:78:LEU:HD23	1:G:92:CYS:HB2	1.97	0.47
3:F:1524:GLU:HG2	3:F:1527:ARG:HH11	1.80	0.46
2:B:47:LEU:HA	2:B:58:VAL:HG21	1.98	0.45
3:C:1438:PHE:HD2	3:C:1618:VAL:HG21	1.81	0.45
1:G:7:SER:HB2	1:G:21:SER:HB2	1.99	0.45
3:X:1515:VAL:HG22	3:X:1584:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLU:HA	1:A:64:LYS:HE3	1.98	0.45
1:D:168:ALA:HB2	1:D:178:LEU:HD23	1.99	0.45
2:B:147:GLN:HB3	2:B:154:LEU:HD11	1.98	0.44
2:E:47:LEU:HA	2:E:58:VAL:HG21	1.99	0.44
2:B:122:ASP:HA	2:B:125:LEU:HD12	1.98	0.44
1:H:168:ALA:HB2	1:H:178:LEU:HD23	1.99	0.44
1:H:7:SER:HB2	1:H:21:SER:HB2	1.99	0.44
1:H:188:SER:HB2	1:H:192:GLN:HG3	2.00	0.44
3:C:1510:ALA:HB2	3:C:1589:ASN:HD21	1.82	0.44
1:D:7:SER:HB3	1:D:21:SER:HB2	1.99	0.44
2:I:19:VAL:HG21	2:I:78:LEU:HD13	2.00	0.44
2:I:47:LEU:HA	2:I:58:VAL:HG21	2.00	0.44
2:L:47:LEU:HA	2:L:58:VAL:HG21	2.00	0.44
3:F:1560:HIS:CD2	3:F:1579:ILE:HG12	2.52	0.44
1:A:168:ALA:HB2	1:A:178:LEU:HD23	2.00	0.44
1:G:67:PHE:CZ	1:G:82:MET:HG2	2.53	0.43
3:J:1612:LEU:HA	3:J:1615:LEU:HD12	2.00	0.43
1:G:168:ALA:HB2	1:G:178:LEU:HD23	2.00	0.43
2:I:113:PRO:HD3	2:I:198:HIS:CD2	2.53	0.43
1:H:168:ALA:HA	1:H:178:LEU:HB3	2.01	0.43
3:F:1631:ARG:HG2	3:F:1632:GLY:N	2.34	0.43
3:X:1507:ALA:HA	3:X:1590:ARG:HD2	2.00	0.43
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.01	0.43
2:B:113:PRO:HD3	2:B:198:HIS:CD2	2.54	0.43
2:L:113:PRO:HD3	2:L:198:HIS:CD2	2.53	0.42
1:D:40:ALA:HB3	1:D:43:LYS:HB2	2.00	0.42
1:G:200:HIS:CD2	1:G:202:PRO:HD2	2.54	0.42
1:A:168:ALA:HA	1:A:178:LEU:HB3	2.01	0.42
1:H:171:GLN:HA	2:L:160:GLN:HE22	1.84	0.42
3:C:1589:ASN:HB3	3:C:1592:CYS:HB2	2.02	0.42
1:G:168:ALA:HA	1:G:178:LEU:HB3	2.01	0.42
2:I:33:ILE:HD11	2:I:88:CYS:HB2	2.02	0.42
2:L:89:GLN:HE21	2:L:96:PHE:HB3	1.84	0.42
1:H:68:THR:HB	1:H:81:GLN:HB3	2.02	0.42
3:X:1633:GLU:HA	3:X:1634:PRO:HD3	1.97	0.42
3:C:1515:VAL:HG22	3:C:1584:MET:HG2	2.01	0.42
1:D:68:THR:HB	1:D:81:GLN:HB3	2.02	0.42
1:A:7:SER:HB3	1:A:21:SER:HB2	2.01	0.41
1:A:68:THR:HB	1:A:81:GLN:HB3	2.02	0.41
1:D:168:ALA:HA	1:D:178:LEU:HB3	2.02	0.41
3:F:1515:VAL:HG22	3:F:1584:MET:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:149:LYS:HG3	2:I:193:ALA:HB3	2.02	0.41
1:G:6:GLU:H	1:G:105:GLN:HE22	1.67	0.41
3:X:1510:ALA:HB2	3:X:1589:ASN:HD21	1.85	0.41
1:G:87:THR:HG23	1:G:110:THR:HA	2.03	0.41
1:G:116:THR:HA	1:G:146:PHE:O	2.20	0.41
1:H:119:PRO:HD2	1:H:205:THR:HG21	2.02	0.41
1:D:119:PRO:HB3	1:D:145:TYR:HB3	2.01	0.41
3:J:1515:VAL:HG22	3:J:1584:MET:HG2	2.02	0.41
3:X:1589:ASN:OD1	3:X:1601:CYS:HB3	2.21	0.41
3:X:1614:ALA:O	3:X:1618:VAL:HG22	2.21	0.41
2:B:13:ALA:O	2:B:106:ILE:HA	2.21	0.41
1:H:87:THR:HG23	1:H:110:THR:HA	2.03	0.41
2:L:89:GLN:NE2	2:L:96:PHE:HB3	2.36	0.40
1:A:87:THR:HG23	1:A:110:THR:HA	2.04	0.40
3:J:1510:ALA:HB2	3:J:1589:ASN:HD21	1.86	0.40
2:I:124:GLN:HE22	2:I:131:SER:H	1.70	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	211/231 (91%)	202 (96%)	8 (4%)	1 (0%)	29	66
1	D	176/231 (76%)	168 (96%)	6 (3%)	2 (1%)	14	47
1	G	211/231 (91%)	200 (95%)	9 (4%)	2 (1%)	17	53
1	H	213/231 (92%)	203 (95%)	9 (4%)	1 (0%)	29	66
2	B	207/214 (97%)	196 (95%)	10 (5%)	1 (0%)	29	66
2	E	136/214 (64%)	128 (94%)	7 (5%)	1 (1%)	22	58
2	I	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29 66
3	C	210/280 (75%)	201 (96%)	7 (3%)	2 (1%)	15 50
3	F	225/280 (80%)	213 (95%)	10 (4%)	2 (1%)	17 53
3	J	210/280 (75%)	200 (95%)	8 (4%)	2 (1%)	15 50
3	X	227/280 (81%)	213 (94%)	10 (4%)	4 (2%)	8 35
All	All	2446/2900 (84%)	2325 (95%)	101 (4%)	20 (1%)	19 55

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ASP
3	C	1430	GLU
1	G	97	ILE
1	G	144	ASP
3	J	1440	ASN
3	J	1634	PRO
3	X	1562	PRO
2	B	138	ASN
1	D	144	ASP
2	E	138	ASN
3	F	1560	HIS
3	F	1562	PRO
1	H	144	ASP
2	L	138	ASN
2	I	138	ASN
3	X	1560	HIS
3	C	1560	HIS
3	X	1430	GLU
1	D	97	ILE
3	X	1578	VAL

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	174/193 (90%)	169 (97%)	5 (3%)	42	74
1	D	139/193 (72%)	131 (94%)	8 (6%)	20	53
1	G	169/193 (88%)	160 (95%)	9 (5%)	22	56
1	H	177/193 (92%)	167 (94%)	10 (6%)	21	54
2	B	181/187 (97%)	170 (94%)	11 (6%)	18	51
2	E	112/187 (60%)	103 (92%)	9 (8%)	12	38
2	I	175/187 (94%)	167 (95%)	8 (5%)	27	61
2	L	184/187 (98%)	175 (95%)	9 (5%)	25	59
3	C	173/236 (73%)	161 (93%)	12 (7%)	15	46
3	F	180/236 (76%)	168 (93%)	12 (7%)	16	47
3	J	168/236 (71%)	157 (94%)	11 (6%)	17	48
3	X	183/236 (78%)	170 (93%)	13 (7%)	14	44
All	All	2015/2464 (82%)	1898 (94%)	117 (6%)	20	53

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	35	THR
1	A	38	ARG
1	A	98	ARG
1	A	148	GLU
2	B	1	ASP
2	B	7	SER
2	B	10	SER
2	B	12	SER
2	B	90	ARG
2	B	154	LEU
2	B	165	GLU
2	B	169	LYS
2	B	176	SER
2	B	191	VAL
2	B	208	SER
3	C	1432	LEU
3	C	1442	ARG
3	C	1466	ARG
3	C	1473	GLU
3	C	1520	LEU
3	C	1544	LEU

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Mol	Chain	Res	Type
3	C	1547	ARG
3	C	1578	VAL
3	C	1585	LEU
3	C	1590	ARG
3	C	1592	CYS
3	C	1628	ARG
1	D	11	LEU
1	D	20	LEU
1	D	35	THR
1	D	38	ARG
1	D	78	LEU
1	D	83	ARG
1	D	85	GLU
1	D	148	GLU
2	E	7	SER
2	E	10	SER
2	E	33	ILE
2	E	54	ARG
2	E	65	SER
2	E	90	ARG
2	E	106	ILE
2	E	107	LYS
2	E	109	THR
3	F	1465	GLU
3	F	1466	ARG
3	F	1484	ARG
3	F	1520	LEU
3	F	1525	LEU
3	F	1528	SER
3	F	1544	LEU
3	F	1545	ARG
3	F	1547	ARG
3	F	1560	HIS
3	F	1590	ARG
3	F	1592	CYS
1	G	12	VAL
1	G	17	SER
1	G	19	ARG
1	G	35	THR
1	G	38	ARG
1	G	63	PHE
1	G	85	GLU

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Mol	Chain	Res	Type
1	G	148	GLU
1	G	191	THR
1	H	19	ARG
1	H	30	THR
1	H	35	THR
1	H	38	ARG
1	H	61	GLU
1	H	64	LYS
1	H	66	ARG
1	H	71	VAL
1	H	78	LEU
1	H	148	GLU
2	I	7	SER
2	I	10	SER
2	I	22	THR
2	I	45	LYS
2	I	90	ARG
2	I	109	THR
2	I	155	GLN
2	I	183	LYS
3	J	1429	CYS
3	J	1432	LEU
3	J	1436	ARG
3	J	1473	GLU
3	J	1503	SER
3	J	1520	LEU
3	J	1544	LEU
3	J	1547	ARG
3	J	1590	ARG
3	J	1606	GLN
3	J	1630	VAL
2	L	1	ASP
2	L	7	SER
2	L	10	SER
2	L	27	GLN
2	L	78	LEU
2	L	90	ARG
2	L	103	LYS
2	L	194	CYS
2	L	208	SER
3	X	1427	ARG
3	X	1442	ARG

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Mol	Chain	Res	Type
3	X	1467	THR
3	X	1493	GLU
3	X	1508	LEU
3	X	1520	LEU
3	X	1525	LEU
3	X	1544	LEU
3	X	1545	ARG
3	X	1547	ARG
3	X	1551	HIS
3	X	1561	ARG
3	X	1585	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	GLN
1	A	164	HIS
2	B	137	ASN
2	B	138	ASN
2	B	198	HIS
3	C	1456	ASN
3	C	1589	ASN
1	D	13	GLN
1	D	81	GLN
1	D	82(A)	ASN
2	E	138	ASN
3	F	1560	HIS
3	F	1589	ASN
1	H	3	GLN
1	H	76	ASN
1	H	164	HIS
1	H	171	GLN
2	I	124	GLN
2	I	137	ASN
2	I	138	ASN
2	I	198	HIS
2	I	199	GLN
3	J	1487	GLN
3	J	1589	ASN
2	L	27	GLN
2	L	53	ASN

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Mol	Chain	Res	Type
2	L	137	ASN
2	L	138	ASN
2	L	160	GLN
2	L	198	HIS
3	X	1456	ASN

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)

2 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	$\#\|Z\| > 2$
4	NAG	P	1	4,3	14,14,15	0.29	0	17,19,21	0.84	1 (5%)
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.66	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
4	NAG	P	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	1	NAG	C1-O5-C5	2.95	116.19	112.19
4	P	2	NAG	C1-O5-C5	2.03	114.95	112.19

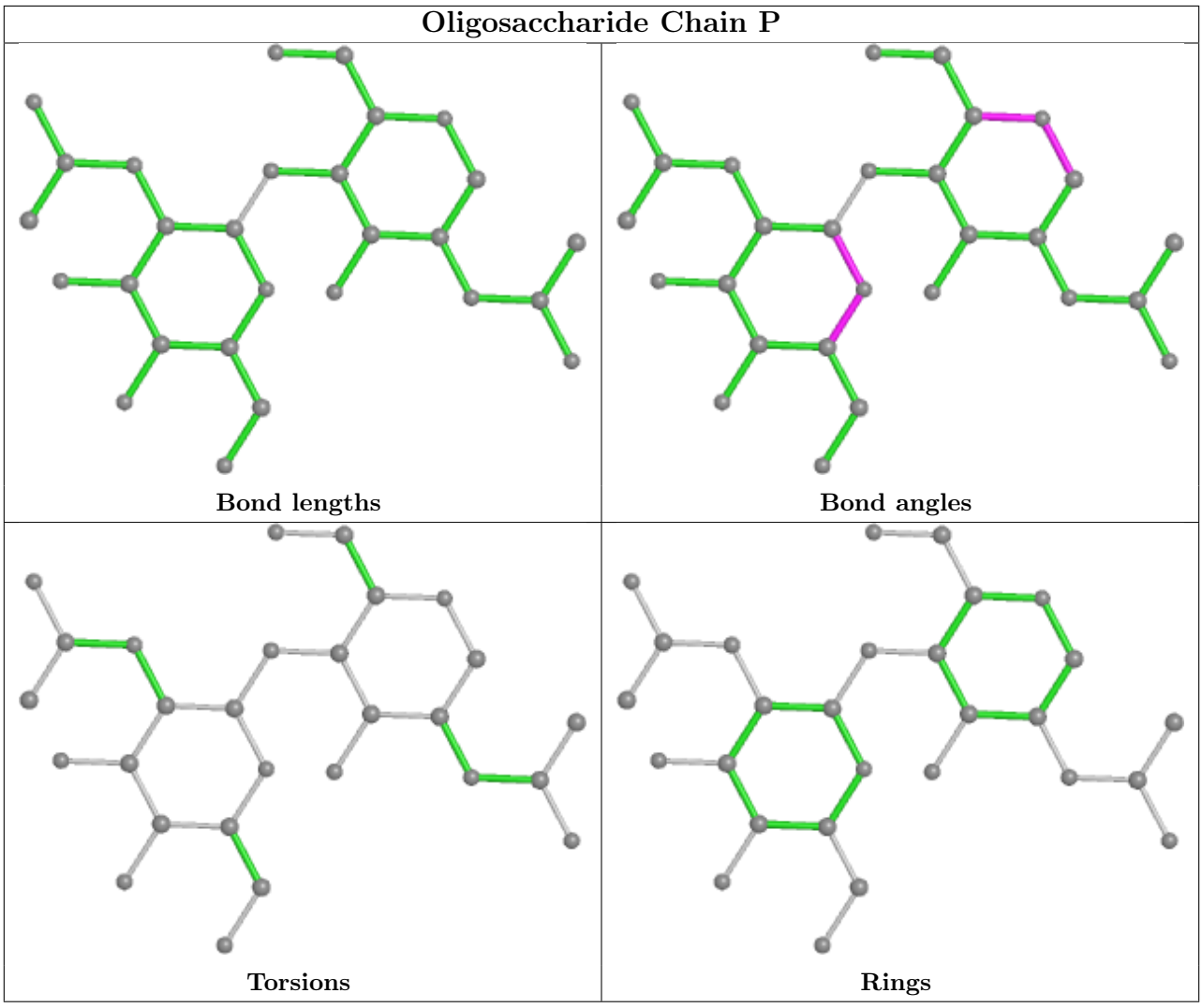
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	1704	3	14,14,15	0.30	0	17,19,21	0.77	0
6	NAG	F	1704	3	14,14,15	0.30	0	17,19,21	0.63	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
6	NAG	C	1704	3	-	2/6/23/26	0/1/1/1
6	NAG	F	1704	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1704	NAG	O5-C5-C6-O6
6	F	1704	NAG	O5-C5-C6-O6
6	C	1704	NAG	C4-C5-C6-O6
6	F	1704	NAG	C4-C5-C6-O6

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, 95^{th} 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	215/231 (93%)	0.47	5 (2%) 60 40	31, 45, 60, 78	0
1	D	184/231 (79%)	0.90	25 (13%) 3 1	49, 71, 102, 124	0
1	G	215/231 (93%)	0.77	23 (10%) 6 3	41, 63, 82, 90	0
1	H	217/231 (93%)	0.38	5 (2%) 60 40	25, 40, 59, 88	0
2	B	211/214 (98%)	0.46	11 (5%) 27 16	31, 53, 83, 92	0
2	E	144/214 (67%)	0.66	13 (9%) 9 5	44, 60, 108, 121	0
2	I	211/214 (98%)	1.01	37 (17%) 1 1	41, 61, 99, 108	0
2	L	213/214 (99%)	0.28	0 100 100	27, 45, 62, 84	0
3	C	220/280 (78%)	0.44	8 (3%) 42 26	36, 58, 86, 100	0
3	F	229/280 (81%)	0.53	10 (4%) 34 20	36, 54, 74, 96	0
3	J	218/280 (77%)	0.70	26 (11%) 4 2	38, 63, 97, 106	0
3	X	231/280 (82%)	0.31	4 (1%) 70 50	30, 53, 74, 93	0
All	All	2508/2900 (86%)	0.57	167 (6%) 17 9	25, 55, 92, 124	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	127	SER	5.7
1	D	152	VAL	5.5
2	I	208	SER	5.4
2	I	33	ILE	5.0
3	J	1457	PHE	4.8
2	E	129	THR	4.8
1	D	141	LEU	4.6
1	D	197	ASN	4.6
2	E	128	GLY	4.5
1	D	142	VAL	4.3
2	E	130	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	200	HIS	4.3
1	G	123	PRO	4.3
2	I	189	HIS	4.2
1	G	147	PRO	4.1
2	I	148	TRP	4.0
3	J	1612	LEU	3.9
2	I	150	VAL	3.9
1	D	4	LEU	3.9
2	I	158	ASN	3.8
1	D	174	GLY	3.7
2	E	132	VAL	3.7
3	C	1550	ALA	3.6
1	G	112	SER	3.6
2	I	64	GLY	3.6
2	I	65	SER	3.5
1	D	155	ASN	3.5
1	D	151	THR	3.5
2	I	67	TYR	3.5
3	J	1615	LEU	3.5
3	J	1439	ASN	3.5
2	E	28	ASN	3.4
1	D	165	THR	3.4
2	B	196	VAL	3.4
1	G	91	TYR	3.4
2	I	152	ASN	3.3
3	F	1489	CYS	3.3
1	G	211	VAL	3.3
2	E	122	ASP	3.3
2	I	149	LYS	3.2
1	D	173	SER	3.2
3	C	1435	TRP	3.2
1	D	153	SER	3.2
2	I	209	PHE	3.1
1	A	195	ILE	3.1
3	F	1461	ALA	3.1
3	X	1433	GLN	3.1
1	A	138	LEU	3.1
1	G	193	THR	3.1
2	B	2	ILE	3.1
2	E	174	SER	3.1
1	G	93	ALA	3.1
3	F	1611	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	J	1614	ALA	3.0
1	G	145	TYR	3.0
2	I	71	PHE	3.0
3	J	1454	TYR	3.0
2	I	51	ALA	3.0
1	D	154	TRP	2.9
1	G	124	LEU	2.9
2	I	157	GLY	2.9
1	G	190	GLY	2.9
2	B	210	ASN	2.9
1	G	189	LEU	2.9
1	D	74	ALA	2.9
3	X	1407	ASN	2.8
3	J	1391	ALA	2.8
3	J	1526	LEU	2.8
1	D	140	CYS	2.8
3	J	1440	ASN	2.8
1	D	91	TYR	2.8
1	D	73	ASN	2.7
1	A	159	LEU	2.7
3	J	1591	LEU	2.7
1	D	75	LYS	2.7
1	G	20	LEU	2.7
2	E	173	TYR	2.7
3	J	1419	SER	2.7
3	J	1608	ALA	2.7
3	J	1516	LEU	2.7
1	D	194	TYR	2.6
1	H	195	ILE	2.6
2	B	33	ILE	2.6
1	G	119	PRO	2.6
2	I	34	ALA	2.6
3	J	1397	ARG	2.6
1	G	177	SER	2.6
1	D	150	VAL	2.6
2	I	207	LYS	2.6
2	I	141	PRO	2.6
1	G	74	ALA	2.6
3	J	1588	ASP	2.6
2	I	205	VAL	2.6
3	F	1407	ASN	2.6
3	F	1462	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	210	LYS	2.5
1	G	148	GLU	2.5
3	C	1498	GLY	2.5
2	I	200	GLY	2.5
3	J	1436	ARG	2.5
1	D	198	VAL	2.5
3	C	1551	HIS	2.5
2	I	88	CYS	2.5
3	J	1587	ILE	2.5
3	J	1413	TRP	2.5
2	E	95	PRO	2.5
3	J	1418	CYS	2.5
2	I	199	GLN	2.5
1	H	33	TRP	2.5
1	D	181	VAL	2.5
3	F	1405	GLU	2.5
2	I	188	LYS	2.5
2	I	193	ALA	2.4
2	I	168	SER	2.4
2	I	159	SER	2.4
2	I	31	ASN	2.4
2	I	138	ASN	2.4
2	I	153	ALA	2.4
3	F	1526	LEU	2.4
3	C	1591	LEU	2.4
3	F	1460	HIS	2.3
3	C	1413	TRP	2.3
3	X	1413	TRP	2.3
2	E	32	ASN	2.3
3	F	1618	VAL	2.3
1	D	82(C)	LEU	2.3
2	I	154	LEU	2.3
1	D	67	PHE	2.3
2	I	35	TRP	2.3
1	H	159	LEU	2.3
3	J	1441	SER	2.3
2	I	181	LEU	2.3
1	A	69	ILE	2.2
2	I	139	PHE	2.2
1	H	71	VAL	2.2
3	F	1491	THR	2.2
2	B	201	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	176	TYR	2.2
2	B	191	VAL	2.2
1	A	128	SER	2.1
1	G	120	SER	2.1
3	J	1543	SER	2.1
1	G	37	VAL	2.1
2	B	209	PHE	2.1
2	E	48	ILE	2.1
1	G	10	GLY	2.1
2	I	30	GLY	2.1
2	B	96	PHE	2.1
3	J	1621	LEU	2.1
3	J	1544	LEU	2.1
2	B	23	CYS	2.1
2	I	89	GLN	2.1
1	G	108	LEU	2.1
3	X	1499	LEU	2.1
1	D	82(A)	ASN	2.1
3	J	1620	ARG	2.0
3	C	1537	SER	2.0
1	G	146	PHE	2.0
2	I	155	GLN	2.0
3	J	1616	SER	2.0
1	D	107	THR	2.0
2	B	29	VAL	2.0
2	E	96	PHE	2.0
3	J	1546	PHE	2.0
3	C	1516	LEU	2.0
2	B	114	SER	2.0
2	I	186	TYR	2.0

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

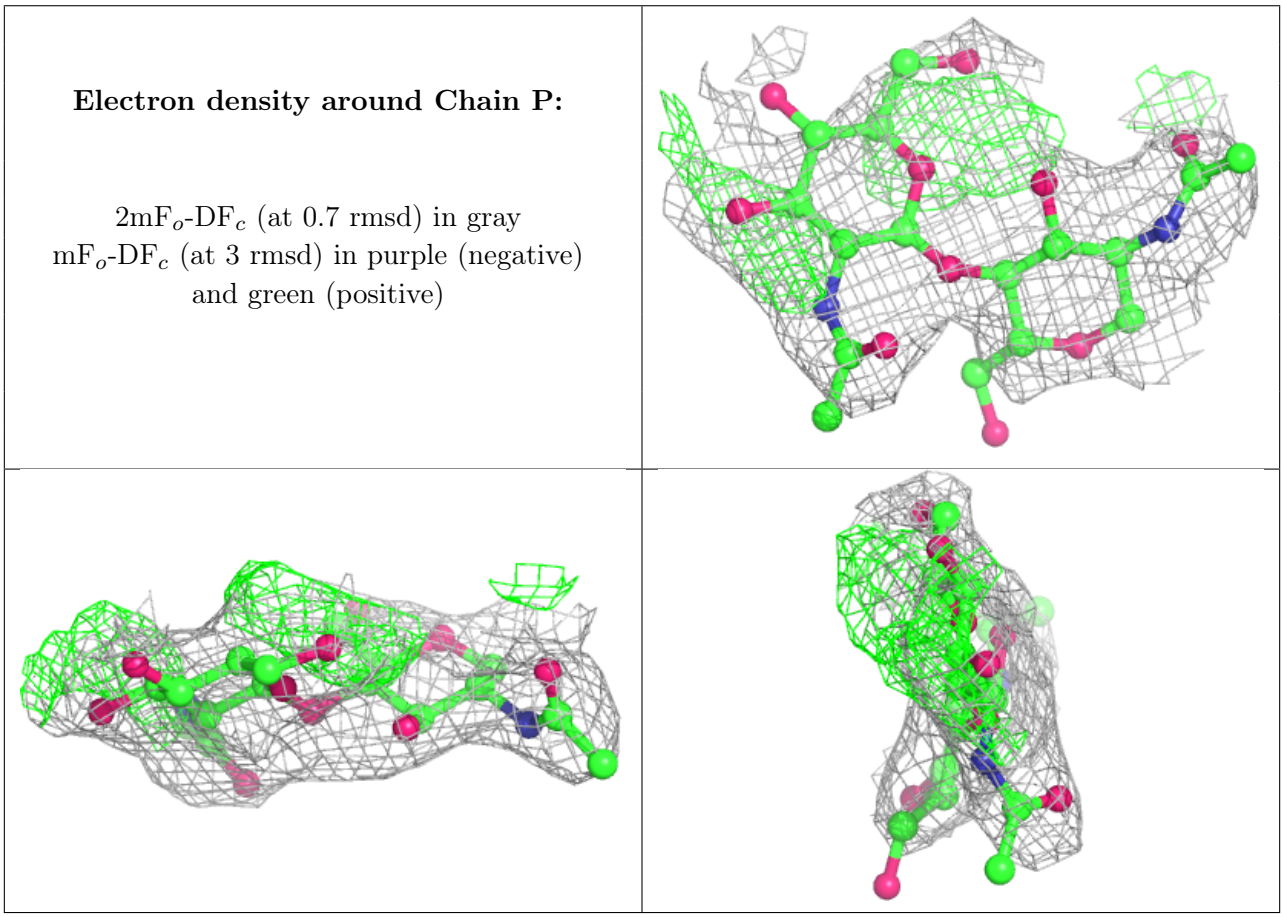
There are no non-standard protein/DNA/RNA residues in this entry.

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. The B-factors column lists the minimum, median, 95^{th} 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
4	NAG	P	2	14/15	0.78	0.35	35,38,41,41	14
4	NAG	P	1	14/15	0.83	0.31	36,41,44,45	14

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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. 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	CA	J	1703	1/1	0.83	0.07	122,122,122,122	0
6	NAG	C	1704	14/15	0.84	0.24	72,73,75,75	0
6	NAG	F	1704	14/15	0.88	0.32	74,76,77,77	0
5	CA	X	1704	1/1	0.90	0.35	84,84,84,84	0
5	CA	F	1703	1/1	0.95	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	1701	1/1	0.96	0.14	47,47,47,47	0
5	CA	J	1702	1/1	0.96	0.14	48,48,48,48	0
5	CA	C	1702	1/1	0.96	0.11	50,50,50,50	0
5	CA	X	1702	1/1	0.96	0.19	60,60,60,60	0
5	CA	C	1703	1/1	0.96	0.16	69,69,69,69	0
5	CA	F	1701	1/1	0.96	0.08	53,53,53,53	0
5	CA	F	1702	1/1	0.96	0.07	61,61,61,61	0
5	CA	X	1703	1/1	0.97	0.11	53,53,53,53	0
5	CA	X	1701	1/1	0.97	0.14	39,39,39,39	0
5	CA	J	1701	1/1	0.99	0.06	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.