



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:58 PM UTC

PDB ID : 6XSW / pdb_00006xsw
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

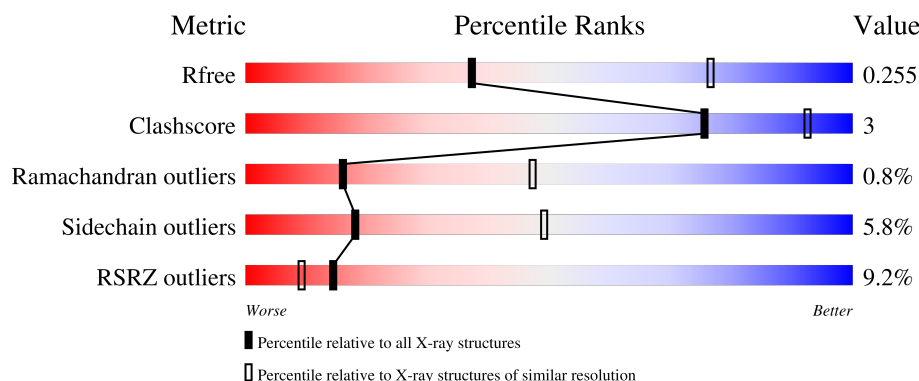
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 $\leq 5\%$. 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	231	15% 81% 11% 7%
1	D	231	15% 68% 12% 20%
1	G	231	9% 78% 14% 7%
1	H	231	2% 81% 13% 6%
2	B	214	7% 84% 14%

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Mol	Chain	Length	Quality of chain
2	E	214	
2	I	214	
2	L	214	
3	C	280	
3	F	280	
3	J	280	
3	X	280	
4	P	2	

2 Entry composition

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.

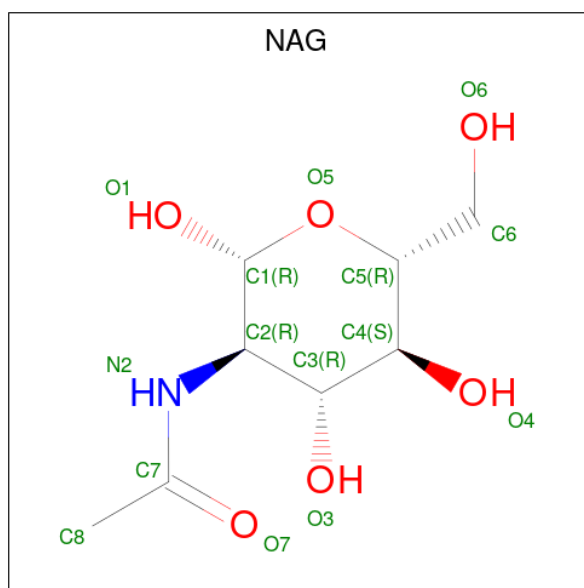


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

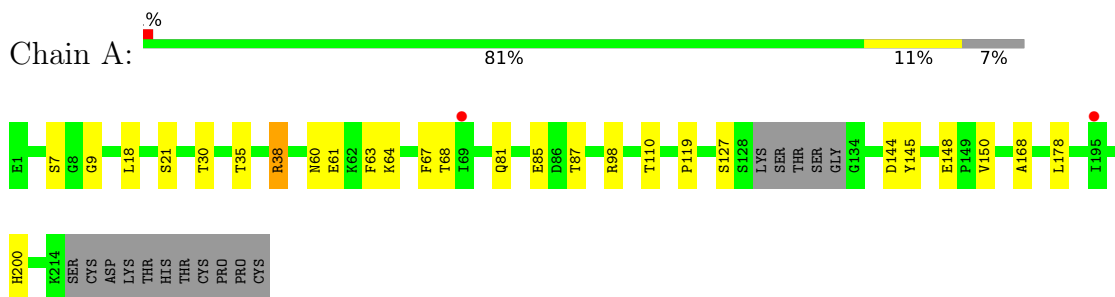
- Molecule 7 is water.

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

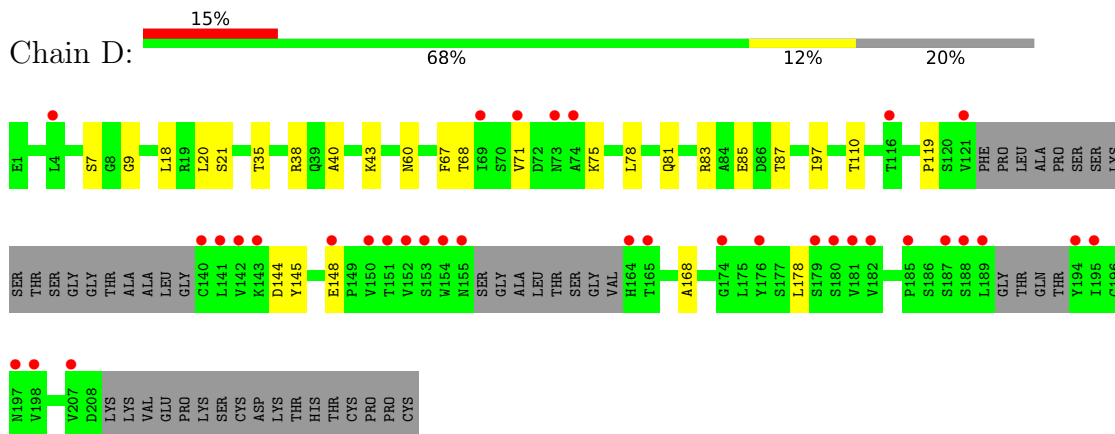
3 Residue-property plots

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.

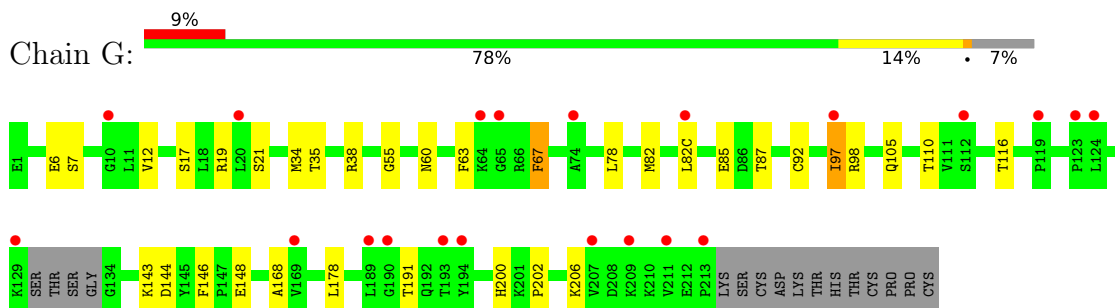
• Molecule 1: Anti-N3 Fab Heavy Chain



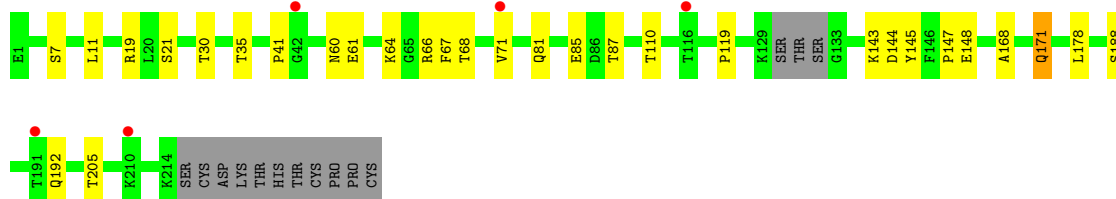
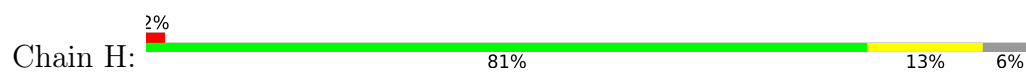
• Molecule 1: Anti-N3 Fab Heavy Chain



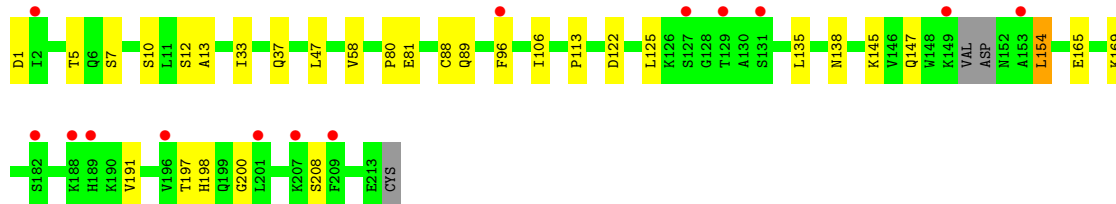
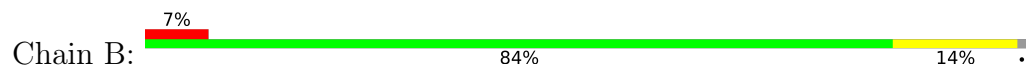
• Molecule 1: Anti-N3 Fab Heavy Chain



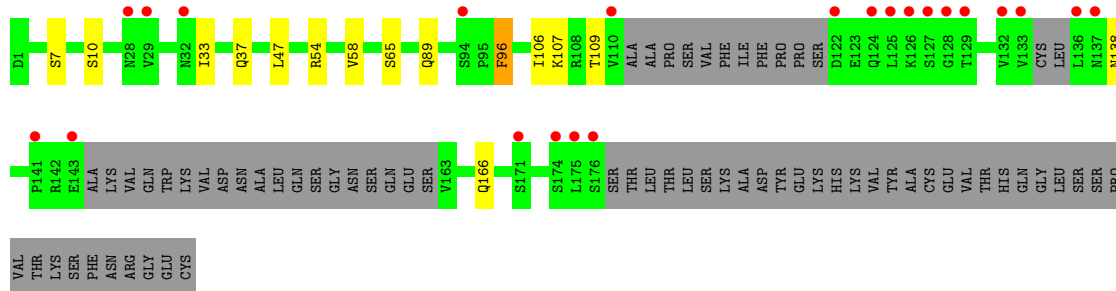
• Molecule 1: Anti-N3 Fab Heavy Chain



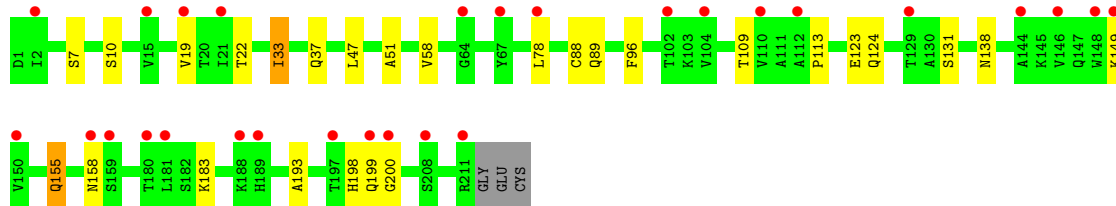
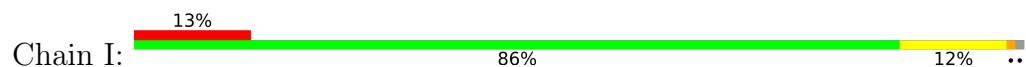
• Molecule 2: Anti-N3 Fab Light Chain



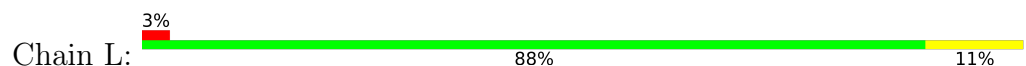
• Molecule 2: Anti-N3 Fab Light Chain

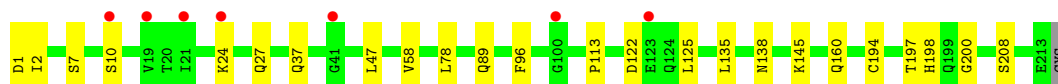


• Molecule 2: Anti-N3 Fab Light Chain

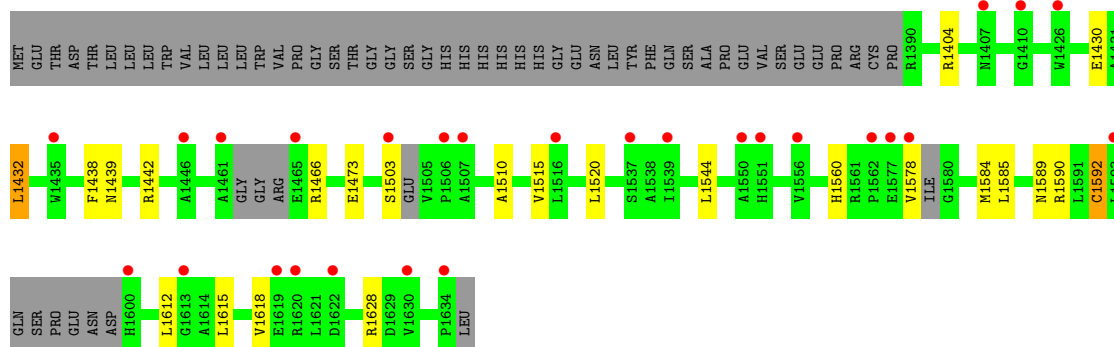


• Molecule 2: Anti-N3 Fab Light Chain

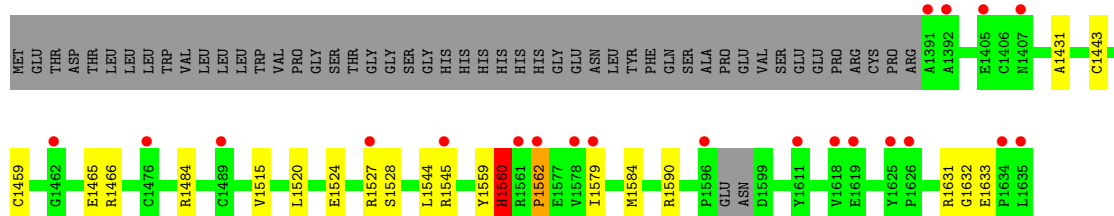
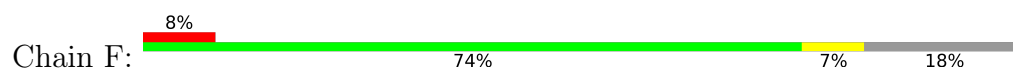




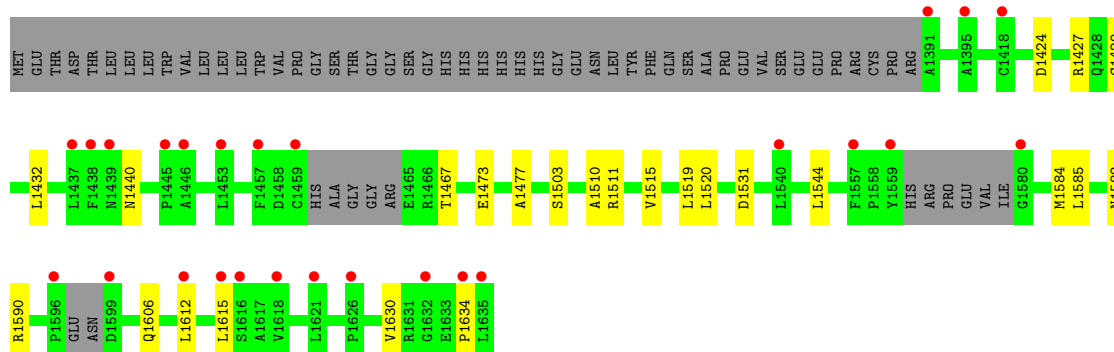
• Molecule 3: Neurogenic locus notch homolog protein 3



• Molecule 3: Neurogenic locus notch homolog protein 3

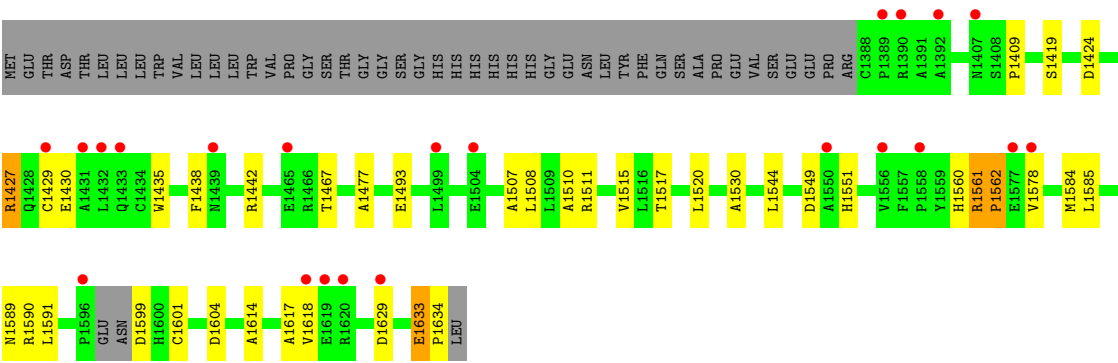


• Molecule 3: Neurogenic locus notch homolog protein 3

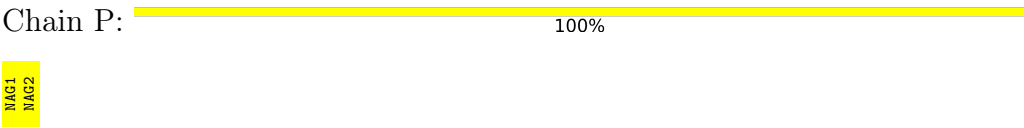


• Molecule 3: Neurogenic locus notch homolog protein 3





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



4 Data and refinement statistics

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 – 2.98 112.66 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.66-2.98) 99.9 (112.66-2.98)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.233 , 0.256 (Not available) , 0.255	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)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for -h,l,k	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.65	0/1653	1.12	5/2257 (0.2%)
1	D	0.66	0/1407	1.12	2/1920 (0.1%)
1	G	0.70	0/1633	1.15	4/2236 (0.2%)
1	H	0.65	0/1671	1.16	7/2278 (0.3%)
2	B	0.69	0/1657	1.10	0/2250
2	E	0.68	0/1091	1.11	4/1483 (0.3%)
2	I	0.71	0/1631	1.10	0/2224
2	L	0.68	0/1676	1.11	0/2278
3	C	0.75	0/1683	1.28	3/2288 (0.1%)
3	F	0.75	0/1754	1.33	6/2390 (0.3%)
3	J	0.77	0/1647	1.35	0/2244
3	X	0.77	0/1778	1.31	4/2420 (0.2%)
All	All	0.71	0/19281	1.20	35/26268 (0.1%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	PRO	CA-C-N	8.05	136.20	121.70
1	H	41	PRO	C-N-CA	8.05	136.20	121.70
1	H	60	ASN	N-CA-C	-6.62	99.12	109.25
3	F	1560	HIS	CA-C-N	6.21	131.36	121.62
3	F	1560	HIS	C-N-CA	6.21	131.36	121.62
3	F	1431	ALA	CA-C-N	5.56	129.16	120.82
3	F	1431	ALA	C-N-CA	5.56	129.16	120.82
3	X	1438	PHE	N-CA-C	-5.53	101.67	109.96
3	X	1429	CYS	N-CA-C	5.47	117.12	108.96
2	E	166	GLN	CA-C-N	5.42	129.38	121.31
2	E	166	GLN	C-N-CA	5.42	129.38	121.31
1	D	60	ASN	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1439	ASN	CA-CB-CG	5.36	117.96	112.60
3	F	1559	TYR	CA-C-N	5.36	131.77	121.54
3	F	1559	TYR	C-N-CA	5.36	131.77	121.54
1	G	67	PHE	CA-CB-CG	5.33	119.13	113.80
1	H	67	PHE	CA-CB-CG	5.33	119.13	113.80
3	X	1599	ASP	CA-CB-CG	5.33	117.93	112.60
2	E	96	PHE	CA-C-N	5.30	128.29	120.82
2	E	96	PHE	C-N-CA	5.30	128.29	120.82
1	A	85	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	67	PHE	CA-CB-CG	5.30	119.10	113.80
3	C	1404	ARG	CA-C-N	5.25	127.84	120.28
3	C	1404	ARG	C-N-CA	5.25	127.84	120.28
1	D	67	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	127	SER	CA-C-N	5.17	131.00	121.70
1	A	127	SER	C-N-CA	5.17	131.00	121.70
3	X	1549	ASP	CA-CB-CG	5.13	117.73	112.60
1	G	55	GLY	CA-C-N	5.09	125.50	120.31
1	G	55	GLY	C-N-CA	5.09	125.50	120.31
1	A	60	ASN	CA-CB-CG	5.09	117.69	112.60
1	G	60	ASN	N-CA-C	-5.08	100.88	108.96
1	H	171	GLN	CA-C-N	5.03	127.72	120.38
1	H	171	GLN	C-N-CA	5.03	127.72	120.38
1	H	60	ASN	CA-CB-CG	5.01	117.61	112.60

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	14	0
1	H	1629	0	1576	10	0
2	B	1621	0	1553	12	0
2	E	1070	0	969	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	109	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 (109) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:MET:HB3	1:G:78:LEU:HD22	1.85	0.57
1:G:82:MET:HE2	1:G:82(C):LEU:HD21	1.88	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	24	58
1	D	176/231 (76%)	168 (96%)	6 (3%)	2 (1%)	11	40
1	G	211/231 (91%)	200 (95%)	9 (4%)	2 (1%)	14	45
1	H	213/231 (92%)	203 (95%)	9 (4%)	1 (0%)	24	58
2	B	207/214 (97%)	196 (95%)	10 (5%)	1 (0%)	24	58
2	E	136/214 (64%)	128 (94%)	7 (5%)	1 (1%)	18	50
2	I	209/214 (98%)	199 (95%)	9 (4%)	1 (0%)	24	58
2	L	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	24	58
3	C	210/280 (75%)	201 (96%)	7 (3%)	2 (1%)	12	42
3	F	225/280 (80%)	213 (95%)	10 (4%)	2 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	210/280 (75%)	200 (95%)	8 (4%)	2 (1%)	12	42
3	X	227/280 (81%)	213 (94%)	10 (4%)	4 (2%)	6	28
All	All	2446/2900 (84%)	2325 (95%)	101 (4%)	20 (1%)	16	47

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 ⓘ

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%)	37	68
1	D	139/193 (72%)	130 (94%)	9 (6%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	169/193 (88%)	158 (94%)	11 (6%)	15	45
1	H	177/193 (92%)	167 (94%)	10 (6%)	19	50
2	B	181/187 (97%)	170 (94%)	11 (6%)	17	47
2	E	112/187 (60%)	104 (93%)	8 (7%)	13	41
2	I	175/187 (94%)	167 (95%)	8 (5%)	24	57
2	L	184/187 (98%)	174 (95%)	10 (5%)	20	51
3	C	173/236 (73%)	161 (93%)	12 (7%)	14	42
3	F	180/236 (76%)	171 (95%)	9 (5%)	22	54
3	J	168/236 (71%)	156 (93%)	12 (7%)	13	41
3	X	183/236 (78%)	171 (93%)	12 (7%)	15	44
All	All	2015/2464 (82%)	1898 (94%)	117 (6%)	18	49

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	81	GLU
2	B	135	LEU
2	B	154	LEU
2	B	165	GLU
2	B	169	LYS
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	1503	SER
3	C	1520	LEU
3	C	1544	LEU

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Mol	Chain	Res	Type
3	C	1578	VAL
3	C	1585	LEU
3	C	1590	ARG
3	C	1592	CYS
3	C	1628	ARG
1	D	20	LEU
1	D	35	THR
1	D	38	ARG
1	D	71	VAL
1	D	75	LYS
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	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	1528	SER
3	F	1544	LEU
3	F	1545	ARG
3	F	1560	HIS
3	F	1590	ARG
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
1	G	143	LYS
1	G	148	GLU
1	G	191	THR
1	G	206	LYS

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Mol	Chain	Res	Type
1	H	19	ARG
1	H	30	THR
1	H	35	THR
1	H	61	GLU
1	H	64	LYS
1	H	66	ARG
1	H	71	VAL
1	H	85	GLU
1	H	143	LYS
1	H	148	GLU
2	I	7	SER
2	I	10	SER
2	I	22	THR
2	I	33	ILE
2	I	109	THR
2	I	123	GLU
2	I	155	GLN
2	I	183	LYS
3	J	1429	CYS
3	J	1432	LEU
3	J	1467	THR
3	J	1473	GLU
3	J	1503	SER
3	J	1511	ARG
3	J	1520	LEU
3	J	1544	LEU
3	J	1585	LEU
3	J	1590	ARG
3	J	1606	GLN
3	J	1630	VAL
2	L	1	ASP
2	L	2	ILE
2	L	7	SER
2	L	10	SER
2	L	24	LYS
2	L	27	GLN
2	L	78	LEU
2	L	135	LEU
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	1544	LEU
3	X	1551	HIS
3	X	1561	ARG
3	X	1585	LEU
3	X	1591	LEU
3	X	1633	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	58	ASN
1	A	76	ASN
1	A	164	HIS
2	B	32	ASN
2	B	79	GLN
2	B	89	GLN
2	B	124	GLN
2	B	137	ASN
2	B	155	GLN
2	B	198	HIS
3	C	1394	GLN
3	C	1490	ASN
3	C	1589	ASN
3	C	1606	GLN
1	D	13	GLN
1	D	58	ASN
1	D	76	ASN
2	E	32	ASN
2	E	89	GLN
3	F	1456	ASN
3	F	1469	ASN
3	F	1490	ASN
3	F	1551	HIS
3	F	1560	HIS
3	F	1589	ASN
1	G	58	ASN
1	G	73	ASN

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Mol	Chain	Res	Type
1	G	76	ASN
1	G	164	HIS
1	H	58	ASN
1	H	76	ASN
1	H	81	GLN
1	H	82(A)	ASN
1	H	164	HIS
1	H	171	GLN
2	I	32	ASN
2	I	79	GLN
2	I	124	GLN
2	I	137	ASN
2	I	155	GLN
2	I	158	ASN
2	I	198	HIS
2	I	199	GLN
3	J	1407	ASN
3	J	1469	ASN
3	J	1487	GLN
3	J	1490	ASN
3	J	1534	GLN
3	J	1589	ASN
2	L	3	GLN
2	L	27	GLN
2	L	32	ASN
2	L	37	GLN
2	L	89	GLN
2	L	124	GLN
2	L	137	ASN
2	L	147	GLN
2	L	160	GLN
2	L	166	GLN
2	L	198	HIS
3	X	1487	GLN
3	X	1490	ASN
3	X	1534	GLN
3	X	1560	HIS

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 ⓘ

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	0.30	0	17,19,21	0.86	1 (5%)
4	NAG	P	2	4	14,14,15	0.31	0	17,19,21	0.68	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(°)	Ideal(°)
4	P	1	NAG	C1-O5-C5	2.99	116.19	112.19
4	P	2	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

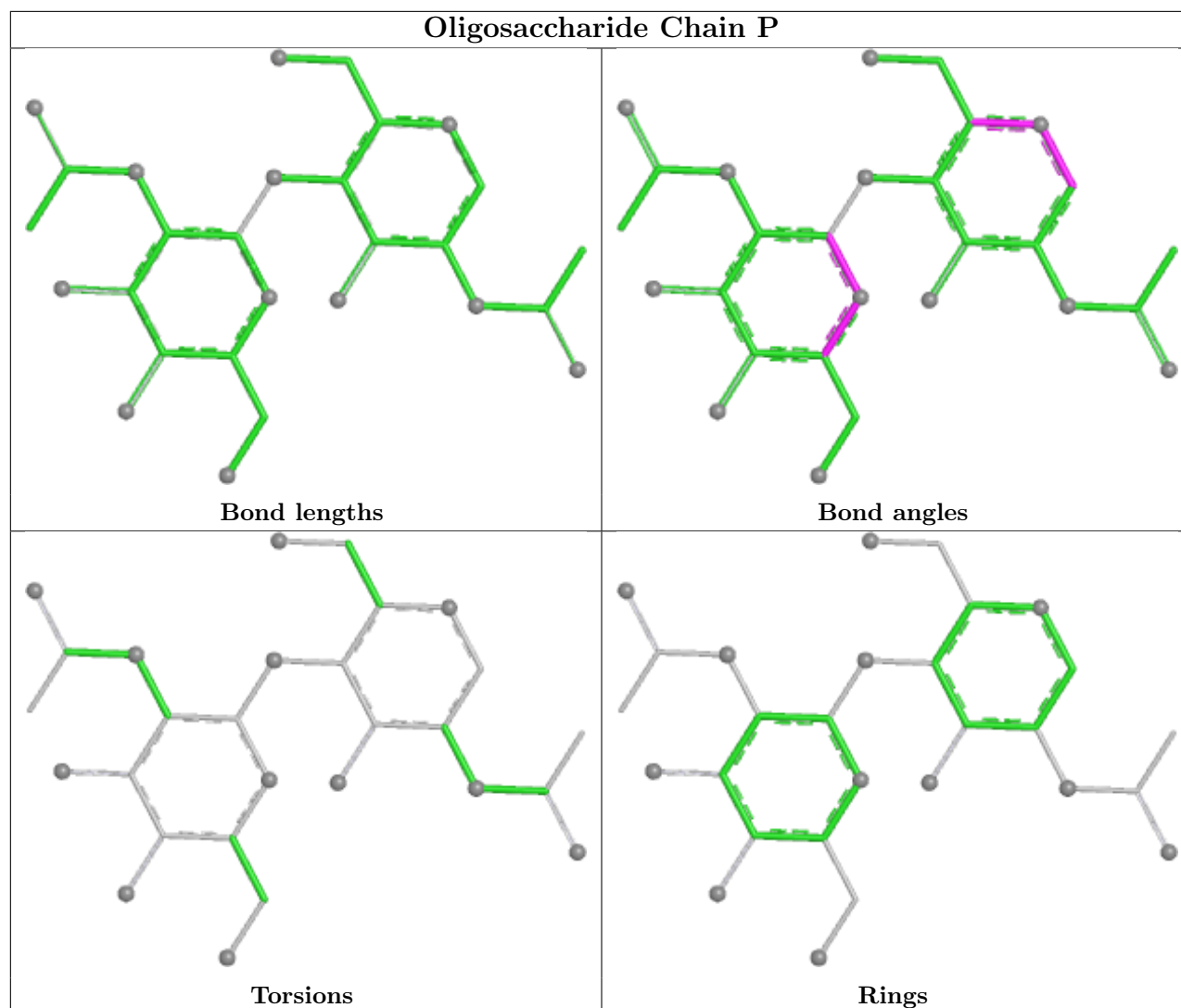
There are no torsion outliers.

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	0.31	0	17,19,21	0.80	0
6	NAG	F	1704	3	14,14,15	0.31	0	17,19,21	0.65	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/231 (93%)	0.41	2 (0%) 81 65	31, 45, 60, 78	0
1	D	184/231 (79%)	1.20	35 (19%) 3 2	49, 71, 102, 124	0
1	G	215/231 (93%)	0.91	21 (9%) 13 8	41, 63, 82, 90	0
1	H	217/231 (93%)	0.39	5 (2%) 61 42	25, 40, 59, 88	0
2	B	211/214 (98%)	0.80	14 (6%) 24 15	31, 53, 83, 92	0
2	E	144/214 (67%)	1.04	22 (15%) 5 3	44, 60, 108, 121	0
2	I	211/214 (98%)	1.05	28 (13%) 7 5	41, 61, 99, 108	0
2	L	213/214 (99%)	0.46	7 (3%) 49 32	27, 45, 62, 84	0
3	C	220/280 (78%)	0.99	27 (12%) 8 6	36, 58, 86, 100	0
3	F	229/280 (81%)	0.71	21 (9%) 14 9	36, 54, 74, 96	0
3	J	218/280 (77%)	1.04	26 (11%) 9 6	38, 63, 97, 106	0
3	X	231/280 (82%)	0.80	22 (9%) 14 9	30, 53, 74, 93	0
All	All	2508/2900 (86%)	0.81	230 (9%) 14 9	25, 55, 92, 124	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	152	VAL	7.1
3	C	1578	VAL	5.8
3	J	1635	LEU	5.3
3	F	1635	LEU	5.1
1	D	121	VAL	4.7
1	D	197	ASN	4.7
3	J	1457	PHE	4.7
2	E	143	GLU	4.6
3	C	1600	HIS	4.6
1	D	181	VAL	4.2
2	E	133	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	189	LEU	4.1
1	D	150	VAL	4.1
2	E	176	SER	4.0
3	J	1599	ASP	3.9
2	E	110	VAL	3.9
3	C	1435	TRP	3.8
2	I	199	GLN	3.8
1	G	97	ILE	3.8
1	D	73	ASN	3.7
3	X	1433	GLN	3.7
1	D	141	LEU	3.7
1	G	211	VAL	3.7
3	J	1438	PHE	3.6
1	D	165	THR	3.6
3	J	1596	PRO	3.5
3	C	1461	ALA	3.5
2	B	2	ILE	3.5
3	C	1622	ASP	3.4
1	G	123	PRO	3.4
3	J	1612	LEU	3.4
2	I	104	VAL	3.4
1	G	74	ALA	3.4
3	F	1596	PRO	3.3
2	E	129	THR	3.3
3	J	1615	LEU	3.3
3	X	1619	GLU	3.2
2	I	200	GLY	3.2
2	E	125	LEU	3.2
3	X	1620	ARG	3.1
1	D	155	ASN	3.1
3	C	1550	ALA	3.1
3	X	1407	ASN	3.1
3	X	1439	ASN	3.1
2	B	149	LYS	3.1
1	D	195	ILE	3.1
1	G	124	LEU	3.0
1	H	71	VAL	3.0
3	F	1407	ASN	3.0
1	G	112	SER	2.9
1	D	198	VAL	2.9
3	J	1453	LEU	2.9
1	D	174	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	J	1446	ALA	2.9
1	G	190	GLY	2.8
2	E	127	SER	2.8
3	C	1410	GLY	2.8
1	D	194	TYR	2.8
2	E	175	LEU	2.8
3	C	1593	LEU	2.8
2	I	129	THR	2.8
1	G	10	GLY	2.8
1	D	185	PRO	2.8
3	F	1562	PRO	2.8
1	D	153	SER	2.8
2	I	208	SER	2.8
1	D	207	VAL	2.8
3	C	1465	GLU	2.7
3	F	1579	ILE	2.7
2	I	158	ASN	2.7
1	H	42	GLY	2.7
2	E	171	SER	2.7
2	I	64	GLY	2.7
3	X	1558	PRO	2.7
1	G	193	THR	2.7
3	X	1596	PRO	2.7
2	B	127	SER	2.7
3	J	1459	CYS	2.7
1	H	116	THR	2.7
1	G	213	PRO	2.7
2	B	153	ALA	2.7
2	B	209	PHE	2.7
3	F	1634	PRO	2.7
2	E	132	VAL	2.7
2	I	188	LYS	2.6
1	H	210	LYS	2.6
2	I	159	SER	2.6
3	C	1634	PRO	2.6
2	I	78	LEU	2.6
2	I	21	ILE	2.6
3	C	1619	GLU	2.6
1	D	180	SER	2.6
1	G	207	VAL	2.6
2	I	19	VAL	2.6
2	I	180	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	1391	ALA	2.6
1	D	142	VAL	2.5
3	X	1618	VAL	2.5
2	B	129	THR	2.5
2	E	137	ASN	2.5
1	D	187	SER	2.5
2	I	146	VAL	2.5
2	L	19	VAL	2.5
3	C	1577	GLU	2.5
3	X	1577	GLU	2.5
2	E	32	ASN	2.5
3	J	1439	ASN	2.5
1	D	116	THR	2.5
3	F	1392	ALA	2.5
3	J	1391	ALA	2.5
2	E	122	ASP	2.5
1	G	82(C)	LEU	2.5
3	C	1551	HIS	2.5
2	E	28	ASN	2.5
1	D	4	LEU	2.4
1	G	209	LYS	2.4
1	D	151	THR	2.4
2	E	29	VAL	2.4
2	I	150	VAL	2.4
2	I	197	THR	2.4
3	J	1418	CYS	2.4
2	B	188	LYS	2.4
1	D	179	SER	2.4
1	D	164	HIS	2.4
3	C	1630	VAL	2.4
1	D	188	SER	2.4
3	C	1503	SER	2.4
2	I	67	TYR	2.4
1	D	74	ALA	2.3
2	I	144	ALA	2.3
2	L	10	SER	2.3
2	I	211	ARG	2.3
3	X	1556	VAL	2.3
3	F	1462	GLY	2.3
2	E	124	GLN	2.3
2	E	174	SER	2.3
2	B	207	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	126	LYS	2.3
3	F	1561	ARG	2.3
2	I	110	VAL	2.3
2	L	100	GLY	2.3
3	F	1405	GLU	2.3
2	I	181	LEU	2.3
3	F	1489	CYS	2.3
3	X	1432	LEU	2.3
2	I	148	TRP	2.3
3	J	1618	VAL	2.3
2	L	123	GLU	2.3
3	X	1392	ALA	2.3
1	D	140	CYS	2.3
2	I	189	HIS	2.3
1	H	191	THR	2.3
2	E	94	SER	2.3
1	D	71	VAL	2.3
3	C	1506	PRO	2.3
3	J	1557	PHE	2.2
3	F	1545	ARG	2.2
1	G	119	PRO	2.2
2	E	141	PRO	2.2
3	J	1445	PRO	2.2
3	J	1580	GLY	2.2
1	D	148	GLU	2.2
1	G	189	LEU	2.2
2	E	136	LEU	2.2
3	C	1407	ASN	2.2
3	X	1499	LEU	2.2
1	D	69	ILE	2.2
3	F	1527	ARG	2.2
2	B	196	VAL	2.2
3	C	1516	LEU	2.2
3	J	1437	LEU	2.2
3	X	1629	ASP	2.2
3	C	1426	TRP	2.2
3	X	1429	CYS	2.2
1	G	194	TYR	2.2
2	B	131	SER	2.2
3	C	1537	SER	2.2
1	D	143	LYS	2.2
1	G	129	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	20	LEU	2.2
3	F	1619	GLU	2.2
2	I	15	VAL	2.2
3	J	1632	GLY	2.2
1	D	176	TYR	2.2
2	E	128	GLY	2.1
3	J	1559	TYR	2.1
3	C	1446	ALA	2.1
3	J	1616	SER	2.1
3	C	1562	PRO	2.1
3	J	1626	PRO	2.1
3	X	1389	PRO	2.1
2	L	24	LYS	2.1
2	B	201	LEU	2.1
3	C	1507	ALA	2.1
3	F	1611	TYR	2.1
3	F	1625	TYR	2.1
3	F	1476	CYS	2.1
2	I	149	LYS	2.1
3	F	1626	PRO	2.1
2	I	112	ALA	2.1
2	L	21	ILE	2.1
3	C	1539	ILE	2.1
2	B	96	PHE	2.1
3	C	1613	GLY	2.1
2	I	102	THR	2.1
3	X	1465	GLU	2.1
1	D	182	VAL	2.0
1	G	169	VAL	2.0
3	F	1618	VAL	2.0
3	X	1578	VAL	2.0
3	J	1634	PRO	2.0
3	J	1540	LEU	2.0
3	J	1621	LEU	2.0
2	I	2	ILE	2.0
3	X	1504	GLU	2.0
1	G	64	LYS	2.0
2	B	182	SER	2.0
2	B	189	HIS	2.0
3	C	1556	VAL	2.0
3	F	1578	VAL	2.0
3	C	1620	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	X	1390	ARG	2.0
1	G	65	GLY	2.0
2	L	41	GLY	2.0
1	A	69	ILE	2.0
1	A	195	ILE	2.0
3	J	1395	ALA	2.0
3	X	1431	ALA	2.0
3	X	1550	ALA	2.0
1	D	154	TRP	2.0

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

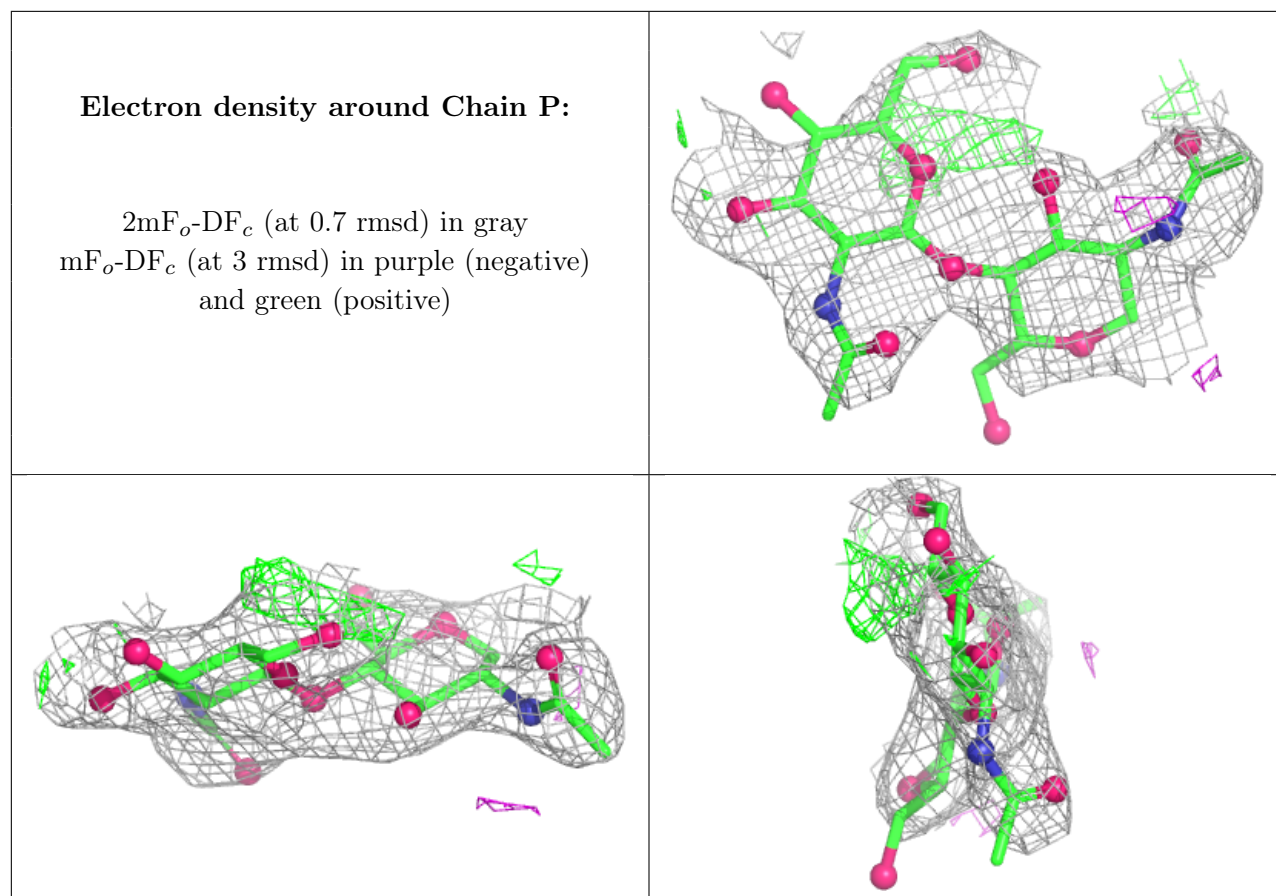
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	NAG	P	1	14/15	-	-	36,41,44,45	14
4	NAG	P	2	14/15	-	-	35,38,41,41	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
6	NAG	C	1704	14/15	0.78	0.13	72,73,75,75	0
6	NAG	F	1704	14/15	0.79	0.10	74,76,77,77	0
5	CA	X	1704	1/1	0.85	0.14	84,84,84,84	0
5	CA	J	1703	1/1	0.96	0.06	122,122,122,122	0
5	CA	C	1703	1/1	0.98	0.07	69,69,69,69	0
5	CA	F	1701	1/1	0.98	0.03	53,53,53,53	0
5	CA	J	1702	1/1	0.99	0.03	48,48,48,48	0
5	CA	C	1701	1/1	0.99	0.04	47,47,47,47	0
5	CA	X	1701	1/1	0.99	0.03	39,39,39,39	0
5	CA	X	1703	1/1	0.99	0.03	53,53,53,53	0
5	CA	F	1702	1/1	0.99	0.02	61,61,61,61	0
5	CA	F	1703	1/1	0.99	0.06	52,52,52,52	0
5	CA	J	1701	1/1	0.99	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	C	1702	1/1	1.00	0.03	50,50,50,50	0
5	CA	X	1702	1/1	1.00	0.09	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.