



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:32 PM EDT

PDB ID : 3L95 / pdb_00003l95
Title : Crystal structure of the human Notch1 Negative Regulatory Region (NRR)
bound to the fab fragment of an antagonist antibody
Authors : Hymowitz, S.G.; de Leon, G.P.
Deposited on : 2010-01-04
Resolution : 2.19 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:

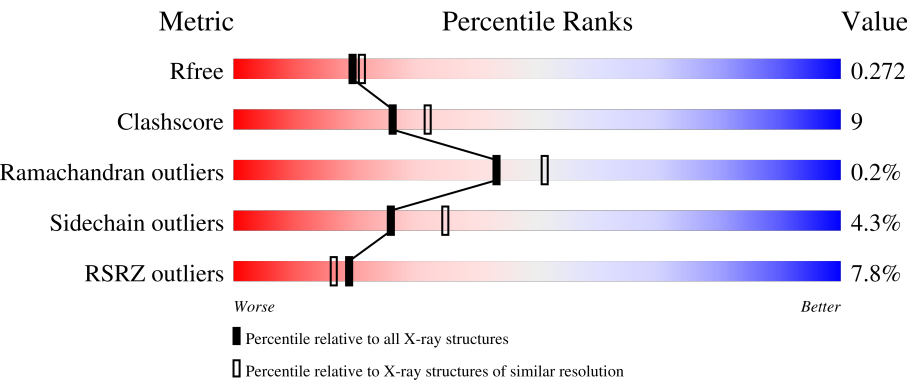
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	214	4% 78% 18% • •
1	L	214	17% 74% 24% • •
2	B	227	2% 88% 8% •
2	H	227	14% 72% 23% • •
3	X	244	5% 77% 15% • 6%

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Mol	Chain	Length	Quality of chain
3	Y	244	3% 72% 15% • 12%
4	C	2	100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10113 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-NRR1 fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1625	1020	269	331	5			
1	L	212	Total	C	N	O	S	0	0	0
			1625	1020	269	331	5			

- Molecule 2 is a protein called anti-NRR1 fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1648	1040	283	319	6			
2	H	219	Total	C	N	O	S	0	0	0
			1643	1037	282	318	6			

- Molecule 3 is a protein called Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	230	Total	C	N	O	S	0	0	0
			1776	1094	309	351	22			
3	Y	215	Total	C	N	O	S	0	1	0
			1676	1037	293	326	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1730	ALA	-	expression tag	UNP P46531
X	1731	ASN	-	expression tag	UNP P46531
X	1732	SER	-	expression tag	UNP P46531
X	1733	HIS	-	expression tag	UNP P46531
X	1734	HIS	-	expression tag	UNP P46531
X	1735	HIS	-	expression tag	UNP P46531
X	1736	HIS	-	expression tag	UNP P46531
X	1737	HIS	-	expression tag	UNP P46531

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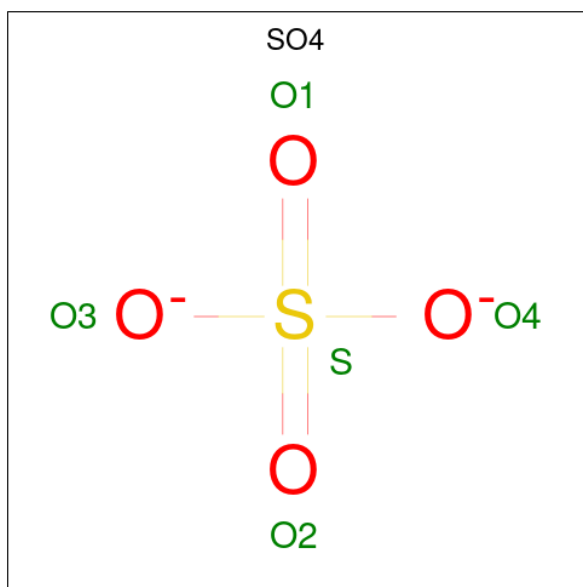
Chain	Residue	Modelled	Actual	Comment	Reference
X	1738	HIS	-	expression tag	UNP P46531
Y	1730	ALA	-	expression tag	UNP P46531
Y	1731	ASN	-	expression tag	UNP P46531
Y	1732	SER	-	expression tag	UNP P46531
Y	1733	HIS	-	expression tag	UNP P46531
Y	1734	HIS	-	expression tag	UNP P46531
Y	1735	HIS	-	expression tag	UNP P46531
Y	1736	HIS	-	expression tag	UNP P46531
Y	1737	HIS	-	expression tag	UNP P46531
Y	1738	HIS	-	expression tag	UNP P46531

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	X	3	Total	Ca	0	0
			3	3		
6	Y	3	Total	Ca	0	0
			3	3		

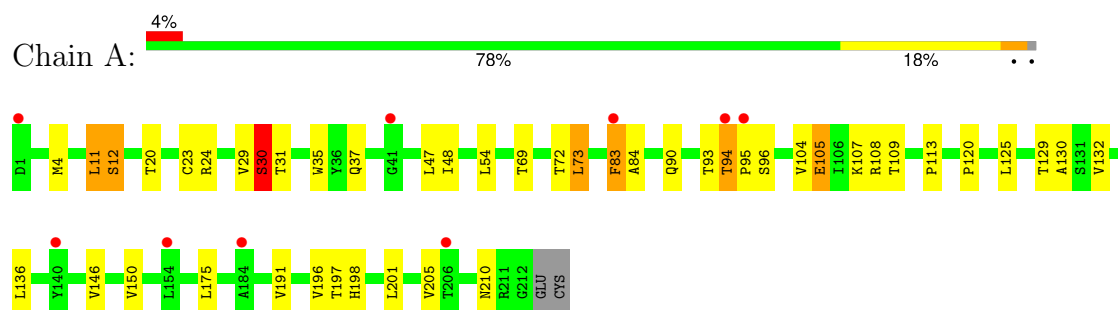
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	14	Total	O	0	0
			14	14		
7	X	37	Total	O	0	0
			37	37		
7	L	4	Total	O	0	0
			4	4		
7	H	3	Total	O	0	0
			3	3		
7	Y	12	Total	O	0	0
			12	12		

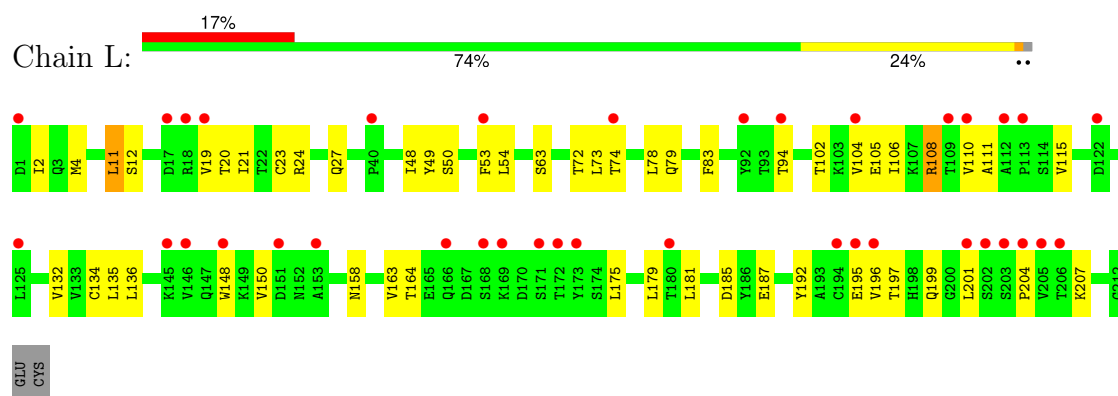
3 Residue-property plots

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.

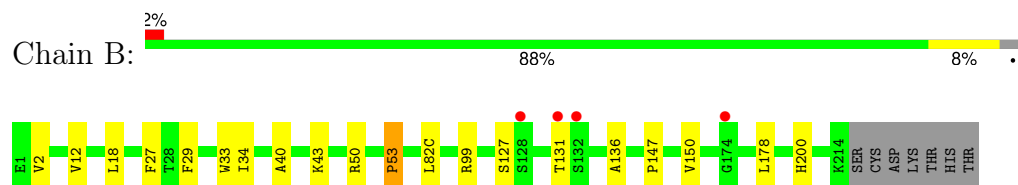
- Molecule 1: anti-NRR1 fab fragment light chain



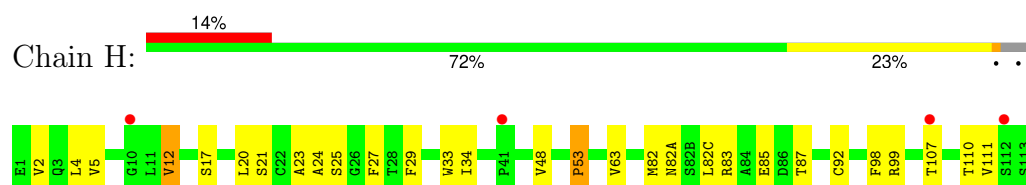
- Molecule 1: anti-NRR1 fab fragment light chain

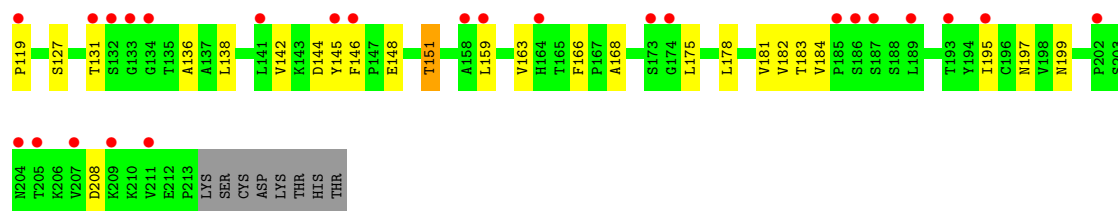


- Molecule 2: anti-NRR1 fab fragment heavy chain

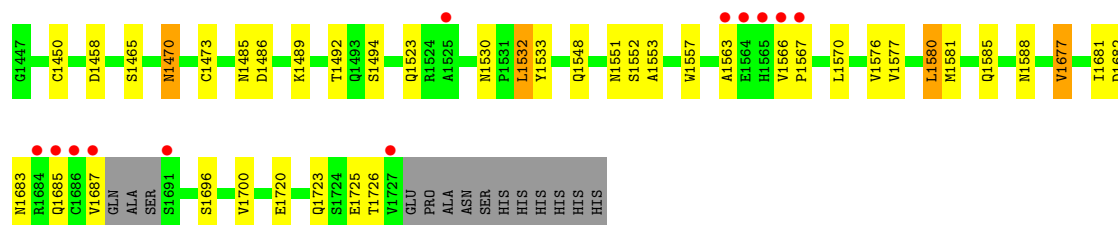
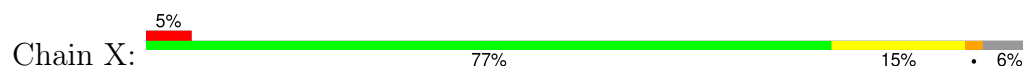


- Molecule 2: anti-NRR1 fab fragment heavy chain

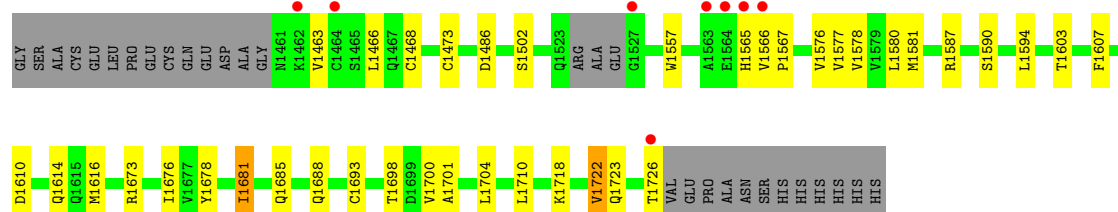




• Molecule 3: Neurogenic locus notch homolog protein 1



• Molecule 3: Neurogenic locus notch homolog protein 1



• 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	46.25Å 163.93Å 179.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.19 30.00 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.19) 97.7 (30.00-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.271 0.227 , 0.272	Depositor DCC
R_{free} test set	6979 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10113	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, SO4

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	0.54	0/1661	0.71	0/2257
1	L	0.46	0/1661	0.66	0/2257
2	B	0.58	0/1691	0.74	1/2307 (0.0%)
2	H	0.49	0/1686	0.67	1/2300 (0.0%)
3	X	0.64	0/1816	0.82	0/2461
3	Y	0.51	0/1719	0.78	0/2330
All	All	0.54	0/10234	0.73	2/13912 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	PRO	N-CA-C	6.18	118.24	110.70
2	H	53	PRO	N-CA-C	5.68	117.63	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1625	0	1578	31	0
1	L	1625	0	1578	53	0
2	B	1648	0	1606	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1643	0	1604	40	0
3	X	1776	0	1605	27	0
3	Y	1676	0	1522	29	0
4	C	28	0	25	3	0
5	B	5	0	0	0	0
6	X	3	0	0	0	0
6	Y	3	0	0	0	0
7	A	11	0	0	0	0
7	B	14	0	0	0	0
7	H	3	0	0	1	0
7	L	4	0	0	1	0
7	X	37	0	0	1	0
7	Y	12	0	0	0	0
All	All	10113	0	9518	183	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 9.

All (183) 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:L:148:TRP:CD2	1:L:179:LEU:HD11	1.91	1.03
1:L:148:TRP:CE2	1:L:179:LEU:HD11	2.00	0.96
3:Y:1576:VAL:CG1	3:Y:1676:ILE:HD11	1.99	0.93
3:Y:1681:ILE:HD12	3:Y:1700:VAL:HG21	1.54	0.88
1:A:90:GLN:NE2	1:A:93:THR:H	1.72	0.87
1:L:21:ILE:HD12	1:L:102:THR:HG21	1.58	0.86
2:H:151:THR:HG22	2:H:199:ASN:HB3	1.61	0.82
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.60	0.81
1:L:135:LEU:CD2	2:H:181:VAL:HG11	2.11	0.81
1:A:136:LEU:HD11	1:A:196:VAL:HG21	1.63	0.80
3:X:1588:ASN:ND2	7:X:19:HOH:O	2.16	0.78
3:Y:1681:ILE:HD11	3:Y:1700:VAL:HG11	1.65	0.77
1:A:20:THR:HG23	1:A:72:THR:CG2	2.17	0.75
2:B:12:VAL:HG21	2:B:82(C):LEU:HD23	1.67	0.74
2:H:33:TRP:CZ2	2:H:99:ARG:HD3	2.24	0.72
1:L:4:MET:HE3	1:L:23:CYS:SG	2.29	0.71
3:Y:1576:VAL:HG12	3:Y:1676:ILE:HD11	1.72	0.71
1:L:135:LEU:HD22	2:H:181:VAL:HG11	1.73	0.71
2:H:159:LEU:CD2	2:H:182:VAL:HG21	2.20	0.71
1:L:20:THR:HG23	1:L:72:THR:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:1581:MET:HE2	3:X:1585:GLN:NE2	2.06	0.69
2:H:33:TRP:CE2	2:H:99:ARG:HD3	2.28	0.69
3:Y:1576:VAL:HG13	3:Y:1676:ILE:HD11	1.73	0.69
1:A:4:MET:HE3	1:A:23:CYS:SG	2.33	0.69
2:H:131:THR:HG22	2:H:136:ALA:HB2	1.74	0.68
3:X:1489:LYS:HD2	4:C:1:NAG:H82	1.75	0.67
2:B:40:ALA:HB3	2:B:43:LYS:HD3	1.77	0.66
1:A:11:LEU:HD12	1:A:11:LEU:C	2.20	0.65
1:A:201:LEU:HD13	1:A:205:VAL:HG23	1.78	0.65
1:L:135:LEU:HD21	2:H:181:VAL:HG11	1.79	0.65
1:A:90:GLN:HE22	1:A:93:THR:H	1.44	0.64
1:L:150:VAL:HG23	1:L:150:VAL:O	1.98	0.63
1:A:20:THR:HG23	1:A:72:THR:HG23	1.81	0.62
3:X:1726:THR:HG22	3:X:1726:THR:O	2.00	0.61
1:L:148:TRP:CE3	1:L:179:LEU:HD11	2.35	0.61
3:X:1570:LEU:HD23	3:X:1682:ASP:HA	1.81	0.61
3:X:1548:GLN:NE2	3:X:1551:ASN:HD22	1.99	0.60
1:L:158:ASN:HD22	1:L:181:LEU:HD21	1.66	0.60
2:B:2:VAL:HG13	2:B:27:PHE:CD2	2.36	0.60
1:L:148:TRP:CE2	1:L:179:LEU:CD1	2.81	0.60
1:L:164:THR:HG23	2:H:166:PHE:CE1	2.37	0.60
1:A:29:VAL:HG11	1:A:90:GLN:HG3	1.84	0.59
1:A:11:LEU:HD11	1:A:104:VAL:HG13	1.84	0.59
3:X:1548:GLN:HE22	3:X:1551:ASN:HD22	1.51	0.59
1:L:78:LEU:HD21	1:L:106:ILE:CD1	2.33	0.59
2:H:2:VAL:HG13	2:H:27:PHE:CD2	2.37	0.58
1:A:146:VAL:HG22	1:A:196:VAL:HG22	1.85	0.58
1:L:163:VAL:HG22	1:L:175:LEU:HD12	1.85	0.58
1:A:30:SER:OG	1:A:31:THR:N	2.32	0.58
2:H:131:THR:HG22	2:H:136:ALA:CB	2.33	0.57
2:H:195:ILE:HD12	2:H:195:ILE:C	2.29	0.57
2:H:99:ARG:NH2	3:Y:1710:LEU:HD13	2.19	0.57
2:B:131:THR:HG22	2:B:136:ALA:HB2	1.85	0.57
1:A:48:ILE:CD1	1:A:54:LEU:HD12	2.35	0.57
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.88	0.56
3:Y:1616:MET:HE2	3:Y:1678:TYR:HB2	1.88	0.56
3:Y:1616:MET:HE2	3:Y:1678:TYR:CB	2.36	0.56
1:A:94:THR:HG23	1:A:95:PRO:HD3	1.87	0.56
1:A:136:LEU:HD11	1:A:196:VAL:CG2	2.33	0.56
2:H:195:ILE:HD12	2:H:195:ILE:O	2.05	0.55
1:L:148:TRP:CG	1:L:179:LEU:HD21	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:ARG:O	2:H:111:VAL:HG21	2.07	0.55
3:Y:1616:MET:HE2	3:Y:1678:TYR:CG	2.42	0.54
2:B:29:PHE:CE1	2:B:34:ILE:HD11	2.43	0.54
1:A:191:VAL:HG22	1:A:210:ASN:ND2	2.22	0.54
2:B:178:LEU:HD12	2:B:178:LEU:C	2.33	0.54
3:X:1576:VAL:HG21	3:X:1725:GLU:HG3	1.91	0.53
2:H:127:SER:O	2:H:131:THR:HG23	2.08	0.52
3:X:1450:CYS:SG	3:X:1470:ASN:OD1	2.66	0.52
2:H:163:VAL:HG22	2:H:182:VAL:HB	1.91	0.52
3:Y:1701:ALA:HB1	3:Y:1722:VAL:HG13	1.90	0.52
1:A:90:GLN:HE21	1:A:93:THR:H	1.56	0.52
2:B:147:PRO:O	2:B:200:HIS:HE1	1.91	0.52
3:X:1530:ASN:OD1	3:X:1532:LEU:HD22	2.09	0.52
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.90	0.52
1:A:136:LEU:HD22	1:A:175:LEU:HD22	1.91	0.52
1:L:195:GLU:OE2	1:L:197:THR:HG23	2.09	0.52
2:H:48:VAL:HG13	2:H:63:VAL:HG21	1.91	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.92	0.51
1:L:148:TRP:CB	1:L:179:LEU:HD21	2.40	0.51
1:L:53:PHE:CE1	3:Y:1463:VAL:HG13	2.45	0.51
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.45	0.51
3:X:1683:ASN:O	3:X:1687:VAL:HG22	2.11	0.51
3:Y:1566:VAL:HG13	3:Y:1567:PRO:HD2	1.93	0.51
2:H:148:GLU:OE2	2:H:168:ALA:HB3	2.11	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CE2	2.46	0.51
3:X:1581:MET:HE2	3:X:1585:GLN:HE21	1.74	0.51
1:L:104:VAL:O	1:L:104:VAL:HG12	2.11	0.50
2:H:12:VAL:O	2:H:111:VAL:HG12	2.11	0.50
2:H:87:THR:OG1	2:H:111:VAL:HG22	2.11	0.50
2:H:146:PHE:HB2	2:H:175:LEU:HD23	1.92	0.50
1:A:93:THR:HG22	1:A:95:PRO:HD2	1.94	0.50
2:H:119:PRO:HB2	2:H:142:VAL:HG13	1.94	0.50
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.47	0.49
3:Y:1681:ILE:CD1	3:Y:1700:VAL:HG11	2.38	0.49
3:X:1557:TRP:HB3	3:X:1685:GLN:HE22	1.76	0.49
2:H:4:LEU:HD23	2:H:92:CYS:SG	2.52	0.49
2:H:5:VAL:HB	2:H:23:ALA:HB3	1.94	0.49
2:H:20:LEU:HD22	2:H:107:THR:HG21	1.95	0.48
1:A:150:VAL:O	1:A:150:VAL:HG13	2.12	0.48
2:B:33:TRP:CE2	2:B:99:ARG:HD2	2.47	0.48
1:L:48:ILE:HD11	1:L:54:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:1552:SER:HA	3:X:1557:TRP:CZ3	2.47	0.48
1:L:108:ARG:NH1	1:L:111:ALA:HB2	2.29	0.48
1:L:63:SER:O	1:L:73:LEU:HD12	2.14	0.48
2:H:138:LEU:HD21	2:H:184:VAL:HG21	1.95	0.47
3:Y:1610:ASP:OD2	3:Y:1614:GLN:N	2.46	0.47
1:A:191:VAL:HG22	1:A:210:ASN:HD21	1.80	0.47
1:L:53:PHE:HE1	3:Y:1463:VAL:HG13	1.80	0.47
1:L:134:CYS:HB2	1:L:148:TRP:CH2	2.49	0.47
1:L:150:VAL:HG12	1:L:192:TYR:CD1	2.49	0.47
1:A:11:LEU:O	1:A:105:GLU:HG2	2.14	0.46
1:L:48:ILE:CD1	1:L:54:LEU:HD12	2.45	0.46
2:H:117:LYS:HZ1	2:H:144:ASP:HB3	1.80	0.46
3:X:1681:ILE:HG13	3:X:1700:VAL:HG21	1.98	0.46
2:B:34:ILE:HD12	2:B:53:PRO:HG3	1.98	0.46
1:L:2:ILE:HD11	1:L:27:GLN:HE21	1.81	0.46
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.98	0.46
2:H:114:ALA:HB1	7:H:224:HOH:O	2.16	0.45
1:L:11:LEU:C	1:L:11:LEU:HD12	2.42	0.45
1:L:115:VAL:HG13	1:L:207:LYS:HG3	1.98	0.45
1:L:136:LEU:HD21	1:L:196:VAL:HG13	1.99	0.45
1:L:150:VAL:O	1:L:150:VAL:CG2	2.63	0.45
2:B:40:ALA:HB3	2:B:43:LYS:CD	2.46	0.45
1:L:136:LEU:HD21	1:L:196:VAL:CG1	2.47	0.45
3:Y:1580:LEU:HD11	3:Y:1673:ARG:NE	2.32	0.45
1:A:20:THR:CG2	1:A:72:THR:HG23	2.45	0.45
2:H:34:ILE:HD12	2:H:53:PRO:HG3	1.99	0.45
1:L:132:VAL:HB	1:L:179:LEU:HD13	1.98	0.44
3:Y:1704:LEU:HD12	3:Y:1722:VAL:HG21	1.99	0.44
3:Y:1577:VAL:HG22	3:Y:1722:VAL:HG23	1.98	0.44
2:B:50:ARG:HD2	2:B:50:ARG:C	2.42	0.44
3:X:1553:ALA:HB2	3:X:1557:TRP:CZ2	2.53	0.44
1:L:11:LEU:HD12	1:L:12:SER:N	2.33	0.43
3:X:1557:TRP:CB	3:X:1685:GLN:HE22	2.31	0.43
1:L:110:VAL:HG23	1:L:110:VAL:O	2.19	0.43
1:L:78:LEU:C	1:L:79:GLN:HE21	2.26	0.43
3:Y:1557:TRP:CD1	3:Y:1685:GLN:HE21	2.36	0.43
3:Y:1587:ARG:O	3:Y:1590:SER:HB2	2.19	0.43
3:X:1489:LYS:CD	4:C:1:NAG:H82	2.46	0.42
3:X:1532:LEU:HD23	3:X:1533:TYR:CD1	2.54	0.42
1:L:48:ILE:HD13	1:L:54:LEU:HA	2.00	0.42
1:L:78:LEU:HD21	1:L:106:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:148:TRP:CZ2	1:L:179:LEU:HD11	2.51	0.42
3:Y:1594:LEU:HD11	3:Y:1607:PHE:CD2	2.54	0.42
3:Y:1580:LEU:HD23	3:Y:1718:LYS:HE2	2.01	0.42
3:Y:1603:THR:HG21	3:Y:1681:ILE:HG23	2.01	0.42
2:H:29:PHE:CE1	2:H:34:ILE:HD11	2.54	0.42
2:H:98:PHE:HB2	3:Y:1466:LEU:HD11	1.99	0.42
3:X:1532:LEU:HD23	3:X:1533:TYR:CE1	2.54	0.42
3:X:1696:SER:HB3	4:C:2:NAG:H83	2.01	0.42
1:L:108:ARG:HH12	1:L:111:ALA:HB2	1.85	0.42
3:Y:1468:CYS:O	3:Y:1473:CYS:HB2	2.20	0.42
3:Y:1578:VAL:CG2	3:Y:1676:ILE:HD13	2.50	0.42
1:L:136:LEU:HD12	1:L:136:LEU:N	2.34	0.42
1:A:35:TRP:CE3	1:A:73:LEU:HD12	2.54	0.42
3:X:1580:LEU:CD2	3:X:1720:GLU:HB3	2.50	0.42
2:H:151:THR:CG2	2:H:199:ASN:HB3	2.42	0.42
3:X:1458:ASP:OD1	3:X:1458:ASP:C	2.63	0.41
3:X:1566:VAL:HG13	3:X:1567:PRO:HD2	2.01	0.41
1:L:20:THR:OG1	1:L:74:THR:HG22	2.20	0.41
1:L:24:ARG:HD2	7:L:215:HOH:O	2.19	0.41
1:L:148:TRP:HB3	1:L:179:LEU:HD21	2.01	0.41
1:L:20:THR:HG23	1:L:72:THR:CG2	2.45	0.41
2:H:145:TYR:OH	2:H:178:LEU:HD23	2.20	0.41
1:A:83:PHE:O	1:A:84:ALA:HB2	2.21	0.41
2:B:127:SER:O	2:B:131:THR:HG23	2.21	0.41
1:L:110:VAL:HG11	1:L:199:GLN:NE2	2.36	0.41
2:H:197:ASN:HD22	2:H:208:ASP:CG	2.28	0.41
3:Y:1578:VAL:HG22	3:Y:1676:ILE:HD13	2.03	0.41
1:L:72:THR:HG22	1:L:74:THR:HG23	2.01	0.41
1:L:49:TYR:CG	3:Y:1466:LEU:HD22	2.56	0.41
1:L:181:LEU:HD22	1:L:185:ASP:OD2	2.20	0.41
2:H:17:SER:HB3	2:H:82(A):ASN:HD22	1.85	0.41
3:Y:1681:ILE:HD12	3:Y:1700:VAL:CG2	2.37	0.41
1:A:129:THR:HG22	1:A:130:ALA:N	2.34	0.41
1:A:24:ARG:HA	1:A:69:THR:O	2.22	0.40
3:X:1485:ASN:O	3:X:1486:ASP:C	2.63	0.40
3:X:1492:THR:HG22	3:X:1494:SER:H	1.85	0.40
1:A:11:LEU:HD12	1:A:12:SER:N	2.36	0.40
3:X:1577:VAL:HB	3:X:1677:VAL:HG22	2.02	0.40
1:L:135:LEU:C	1:L:136:LEU:HD12	2.46	0.40
1:L:11:LEU:HD21	1:L:19:VAL:HG11	2.04	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	210/214 (98%)	202 (96%)	7 (3%)	1 (0%)	24	27
1	L	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	B	218/227 (96%)	215 (99%)	3 (1%)	0	100	100
2	H	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
3	X	226/244 (93%)	219 (97%)	6 (3%)	1 (0%)	30	34
3	Y	212/244 (87%)	206 (97%)	5 (2%)	1 (0%)	24	27
All	All	1293/1370 (94%)	1245 (96%)	45 (4%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	X	1563	ALA
1	A	30	SER
3	Y	1486	ASP

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	186/188 (99%)	173 (93%)	13 (7%)	14	16
1	L	186/188 (99%)	178 (96%)	8 (4%)	26	35
2	B	182/190 (96%)	180 (99%)	2 (1%)	65	79
2	H	182/190 (96%)	175 (96%)	7 (4%)	29	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	196/208 (94%)	188 (96%)	8 (4%)	27	37
3	Y	186/208 (89%)	176 (95%)	10 (5%)	20	25
All	All	1118/1172 (95%)	1070 (96%)	48 (4%)	26	35

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	SER
1	A	30	SER
1	A	73	LEU
1	A	83	PHE
1	A	94	THR
1	A	96	SER
1	A	105	GLU
1	A	107	LYS
1	A	108	ARG
1	A	109	THR
1	A	125	LEU
1	A	197	THR
2	B	18	LEU
2	B	150	VAL
3	X	1465	SER
3	X	1470	ASN
3	X	1473	CYS
3	X	1523	GLN
3	X	1532	LEU
3	X	1580	LEU
3	X	1677	VAL
3	X	1723	GLN
1	L	11	LEU
1	L	50	SER
1	L	83	PHE
1	L	94	THR
1	L	105	GLU
1	L	108	ARG
1	L	187	GLU
1	L	201	LEU
2	H	12	VAL
2	H	21	SER
2	H	25	SER

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Mol	Chain	Res	Type
2	H	85	GLU
2	H	110	THR
2	H	151	THR
2	H	183	THR
3	Y	1502	SER
3	Y	1565	HIS
3	Y	1581	MET
3	Y	1681	ILE
3	Y	1688	GLN
3	Y	1693	CYS
3	Y	1698	THR
3	Y	1722	VAL
3	Y	1723	GLN
3	Y	1726	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	90	GLN
1	A	138	ASN
1	A	155	GLN
1	A	198	HIS
1	A	199	GLN
1	A	210	ASN
2	B	13	GLN
2	B	35	HIS
2	B	39	GLN
2	B	55	ASN
2	B	82(A)	ASN
2	B	171	GLN
2	B	200	HIS
3	X	1470	ASN
3	X	1523	GLN
3	X	1548	GLN
3	X	1551	ASN
3	X	1585	GLN
3	X	1685	GLN
3	X	1692	GLN
3	X	1695	GLN
1	L	27	GLN
1	L	38	GLN

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Mol	Chain	Res	Type
1	L	79	GLN
1	L	124	GLN
1	L	155	GLN
1	L	158	ASN
2	H	39	GLN
2	H	82(A)	ASN
2	H	171	GLN
3	Y	1493	GLN
3	Y	1505	HIS
3	Y	1511	ASN
3	Y	1523	GLN
3	Y	1535	GLN
3	Y	1551	ASN
3	Y	1683	ASN
3	Y	1688	GLN
3	Y	1692	GLN
3	Y	1723	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	C	1	3,4	14,14,15	0.62	0	17,19,21	2.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2	4	14,14,15	0.52	0	17,19,21	1.30	4 (23%)

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	C	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	7.80	122.64	112.19
4	C	1	NAG	O5-C1-C2	3.42	116.58	111.29
4	C	1	NAG	O4-C4-C5	2.92	116.51	109.32
4	C	2	NAG	C1-O5-C5	2.83	115.98	112.19
4	C	2	NAG	C3-C4-C5	2.63	115.01	110.23
4	C	2	NAG	O5-C1-C2	-2.36	107.64	111.29
4	C	2	NAG	C6-C5-C4	-2.11	107.85	113.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

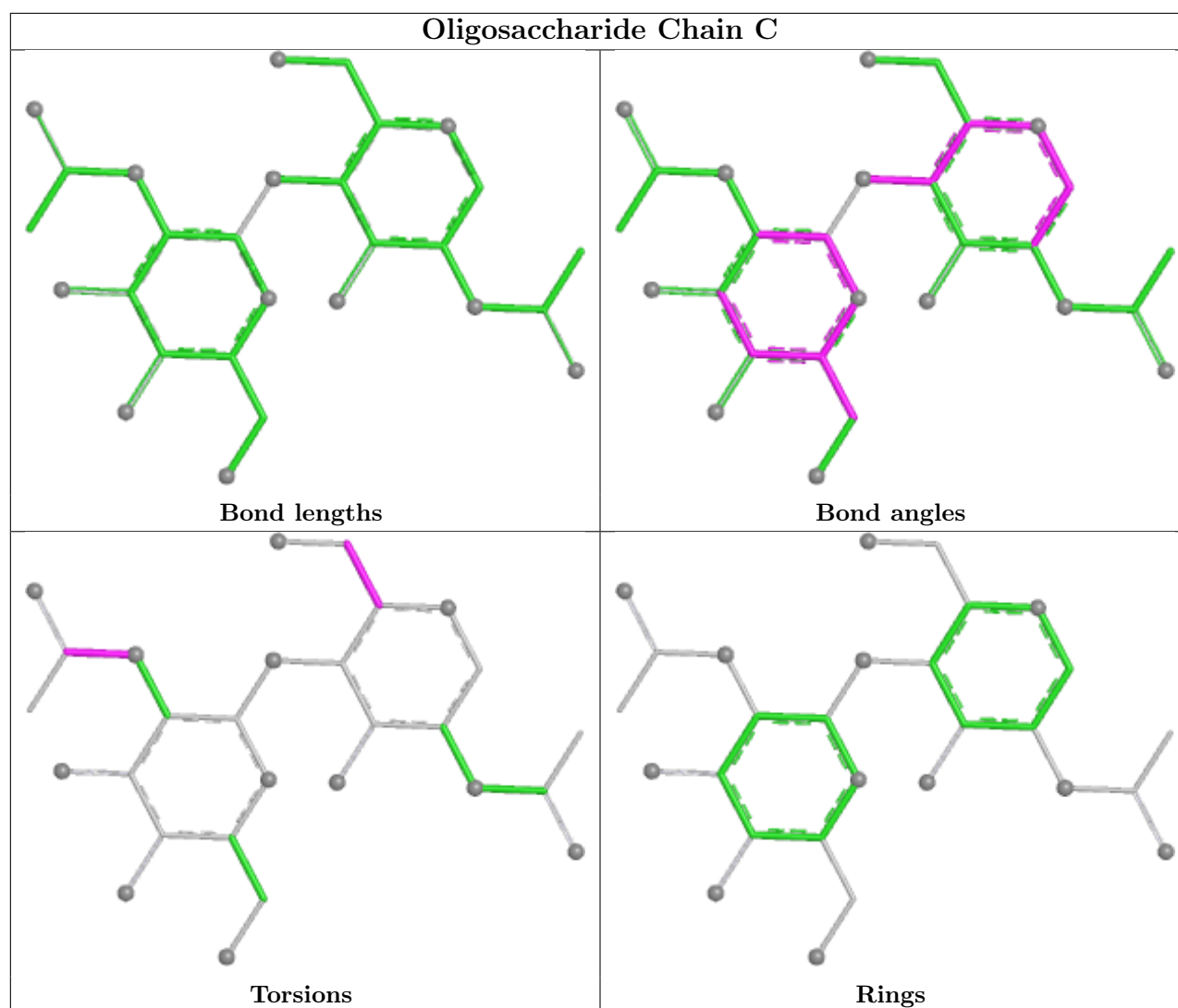
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	1	0
4	C	1	NAG	2	0

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 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
5	SO4	B	222	-	4,4,4	0.31	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/214 (99%)	0.37	9 (4%) 40 37	20, 35, 47, 57	0
1	L	212/214 (99%)	1.12	37 (17%) 4 3	20, 35, 47, 56	0
2	B	220/227 (96%)	0.20	4 (1%) 67 64	17, 30, 46, 57	0
2	H	219/227 (96%)	0.96	32 (14%) 6 4	18, 30, 45, 57	0
3	X	230/244 (94%)	0.09	12 (5%) 33 29	12, 26, 56, 80	0
3	Y	215/244 (88%)	0.19	8 (3%) 45 42	12, 28, 50, 77	1 (0%)
All	All	1308/1370 (95%)	0.48	102 (7%) 19 16	12, 31, 48, 80	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	THR	4.6
1	A	83	PHE	4.2
3	Y	1527	GLY	4.0
2	H	211	VAL	4.0
1	L	201	LEU	3.9
1	L	205	VAL	3.8
1	L	94	THR	3.5
2	B	131	THR	3.4
2	H	189	LEU	3.3
2	H	112	SER	3.3
2	H	133	GLY	3.2
3	Y	1566	VAL	3.2
3	X	1566	VAL	3.2
3	X	1525	ALA	3.2
2	H	185	PRO	3.2
1	L	112	ALA	3.1
1	L	146	VAL	3.1
2	H	187	SER	3.1
2	H	132	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	10	GLY	3.0
1	L	109	THR	2.9
2	H	116	THR	2.9
2	B	132	SER	2.9
2	H	134	GLY	2.9
3	Y	1565	HIS	2.9
3	Y	1563	ALA	2.9
3	X	1686	CYS	2.8
1	L	180	THR	2.8
2	B	128	SER	2.8
1	L	153	ALA	2.8
1	L	173	TYR	2.8
1	L	40	PRO	2.8
2	H	202	PRO	2.8
1	L	168	SER	2.7
1	A	1	ASP	2.7
1	L	195	GLU	2.7
1	L	196	VAL	2.7
2	H	207	VAL	2.7
1	L	194	CYS	2.7
2	H	159	LEU	2.7
1	L	110	VAL	2.7
1	L	74	THR	2.6
2	H	204	ASN	2.6
3	Y	1564	GLU	2.6
1	L	122	ASP	2.6
2	H	146	PHE	2.5
1	A	140	TYR	2.5
2	H	158	ALA	2.5
1	L	202	SER	2.5
2	H	145	TYR	2.5
1	A	206	THR	2.5
1	L	125	LEU	2.5
3	X	1565	HIS	2.5
2	H	174	GLY	2.5
2	H	131	THR	2.4
1	L	18	ARG	2.4
2	H	195	ILE	2.4
3	X	1563	ALA	2.4
3	X	1685	GLN	2.4
2	H	41	PRO	2.4
1	L	17	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	X	1687	VAL	2.4
1	L	113	PRO	2.4
2	H	118	GLY	2.3
3	X	1691	SER	2.3
1	A	95	PRO	2.3
1	L	203	SER	2.3
3	X	1564	GLU	2.3
2	H	119	PRO	2.3
1	L	151	ASP	2.3
2	H	141	LEU	2.3
1	L	92	TYR	2.3
1	L	148	TRP	2.3
1	L	206	THR	2.2
3	Y	1726	THR	2.2
3	X	1684	ARG	2.2
2	H	107	THR	2.2
2	H	193	THR	2.2
1	L	166	GLN	2.2
2	H	114	ALA	2.2
1	L	1	ASP	2.2
1	L	53	PHE	2.1
1	L	104	VAL	2.1
3	X	1727	VAL	2.1
1	L	145	LYS	2.1
2	H	205	THR	2.1
1	A	154	LEU	2.1
1	L	172	THR	2.1
1	A	41	GLY	2.1
1	L	19	VAL	2.1
1	L	169	LYS	2.1
3	Y	1462	LYS	2.1
2	H	186	SER	2.1
1	L	204	PRO	2.1
2	B	174	GLY	2.1
2	H	164	HIS	2.0
2	H	209	LYS	2.0
1	L	171	SER	2.0
2	H	173	SER	2.0
1	A	184	ALA	2.0
3	Y	1464	CYS	2.0
3	X	1567	PRO	2.0

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

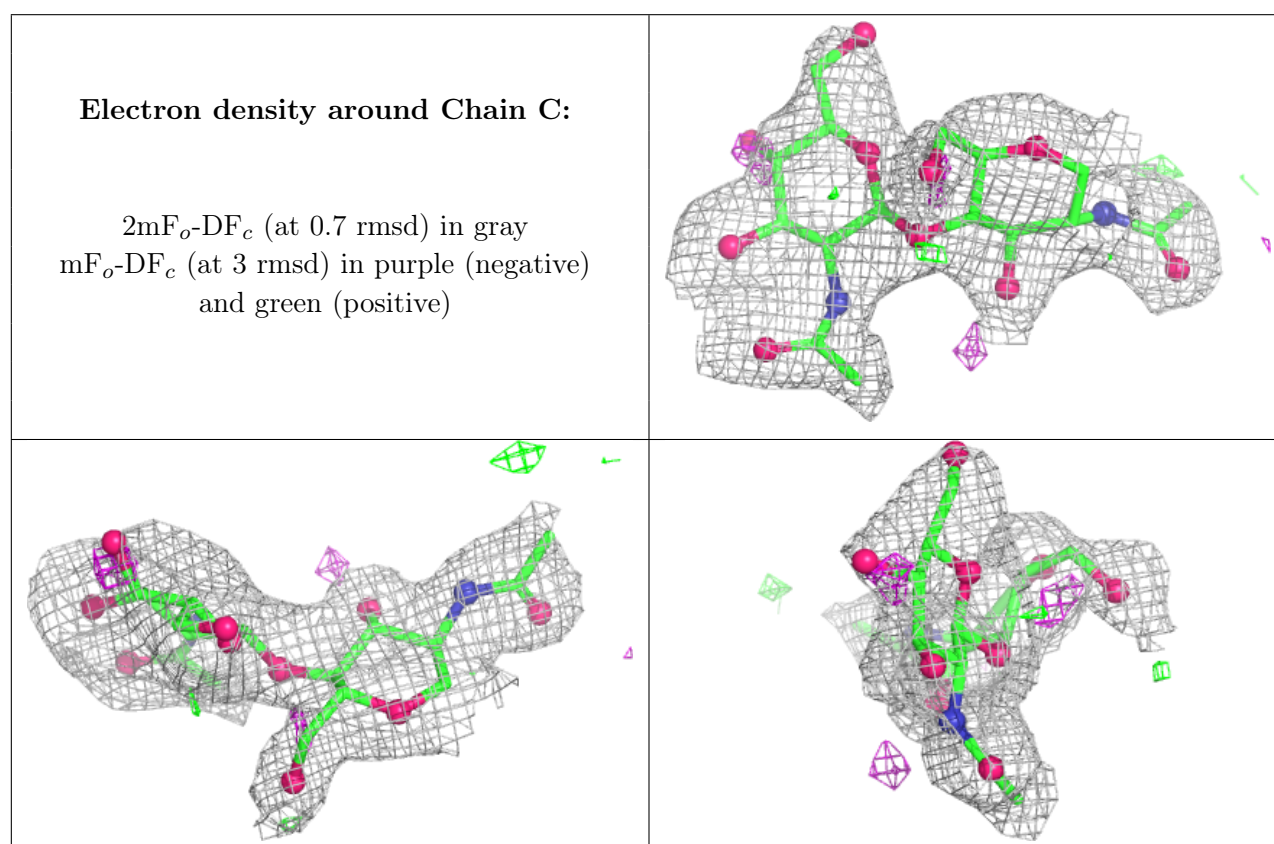
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	31,40,50,50	0
4	NAG	C	2	14/15	-	-	53,56,61,64	0

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($\text{\AA}^2$)	Q<0.9
6	CA	Y	2001	1/1	0.90	0.19	67,67,67,67	0
6	CA	X	2001	1/1	0.97	0.16	43,43,43,43	0
6	CA	Y	2002	1/1	0.98	0.10	21,21,21,21	0
5	SO4	B	222	5/5	0.99	0.11	31,32,32,33	0
6	CA	Y	2003	1/1	0.99	0.10	23,23,23,23	0
6	CA	X	2003	1/1	1.00	0.08	21,21,21,21	0
6	CA	X	2002	1/1	1.00	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.