



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:07 AM UTC

PDB ID : 9YXD / pdb\_00009yxd  
Title : Crystal structure of recombinant human follicle stimulating hormone in complex with an anti-FSH alpha Fab  
Authors : Joseph, J.S.; Kalson, D.; Bakshi, S.  
Deposited on : 2025-10-27  
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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

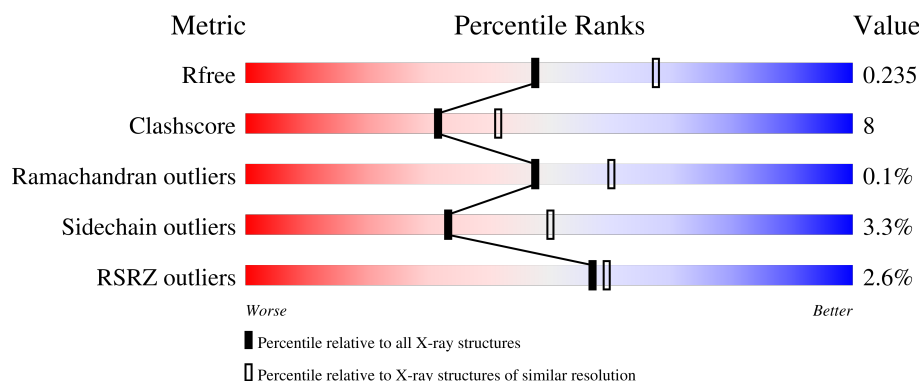
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	92	
2	B	111	
3	C	220	
4	D	225	
5	K	127	

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Mol	Chain	Length	Quality of chain
6	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GOL	D	301	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6146 atoms, of which 27 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 Glycoprotein hormones alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	S	0	0	0
			669	415	116	125	13			

- Molecule 2 is a protein called Follitropin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			823	513	138	160	12			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1663	1039	279	339	6			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	216	Total	C	N	O	S	0	0	0
			1639	1035	272	326	6			

- Molecule 5 is a protein called Ig-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	119	Total	C	N	O	S	0	0	0
			916	569	161	182	4			

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



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

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



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

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula:  $C_8H_{19}NO_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	H	O	0	0
			14	3	8	3		

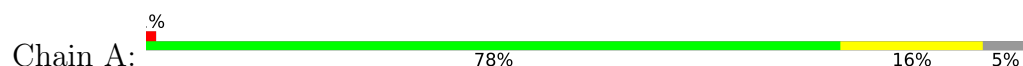
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	45	Total 45	O 45	0	0
10	B	48	Total 48	O 48	0	0
10	C	105	Total 105	O 105	0	0
10	D	84	Total 84	O 84	0	0
10	K	37	Total 37	O 37	0	0

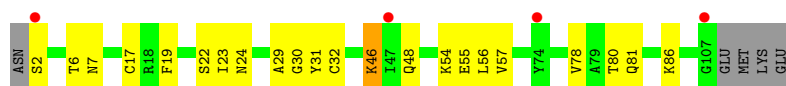
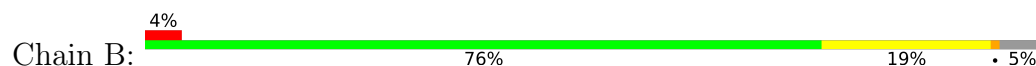
### 3 Residue-property plots [i](#)

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.

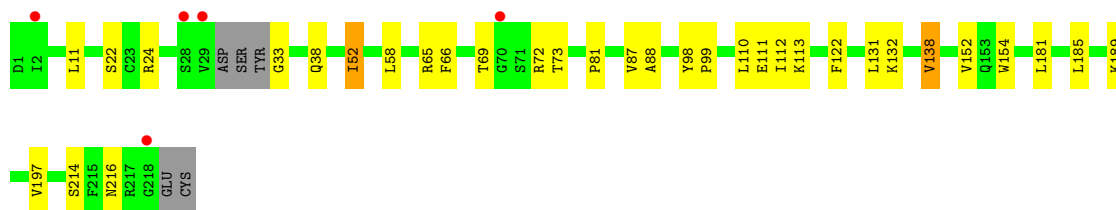
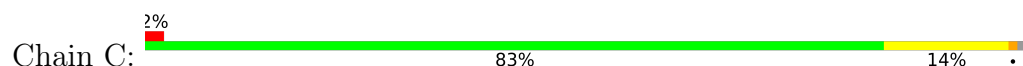
- Molecule 1: Glycoprotein hormones alpha chain



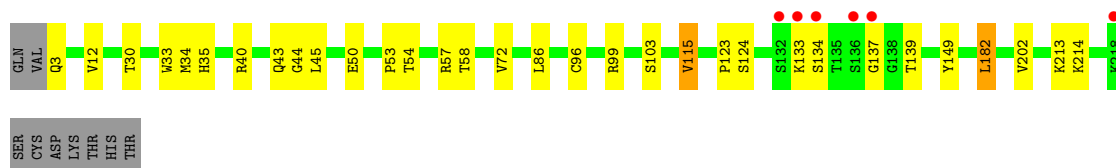
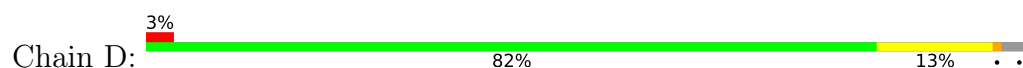
- Molecule 2: Follitropin subunit beta



- Molecule 3: Fab light chain



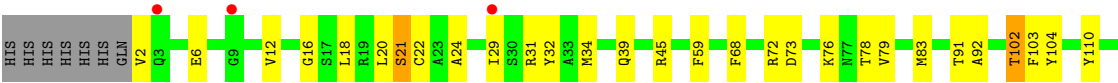
- Molecule 4: Fab heavy chain



- Molecule 5: Ig-like domain-containing protein







S120  
SER

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



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.01Å 101.10Å 161.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 2.29 29.85 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.85-2.29) 98.5 (29.85-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.66 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5084	Depositor
R, $R_{free}$	0.201 , 0.235 0.201 , 0.235	Depositor DCC
$R_{free}$ test set	2814 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: NAG, GOL, BTB

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	0/685	0.54	0/926
2	B	0.33	0/842	0.49	0/1144
3	C	0.34	0/1698	0.52	0/2304
4	D	0.32	0/1681	0.56	0/2289
5	K	0.32	0/935	0.53	0/1264
All	All	0.33	0/5841	0.53	0/7927

There are no bond length outliers.

There are no bond angle outliers.

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	669	0	639	10	0
2	B	823	0	776	18	0
3	C	1663	0	1606	20	0
4	D	1639	0	1598	24	0
5	K	916	0	862	25	0
6	E	28	0	25	2	0
7	A	14	0	13	1	0
7	B	28	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	14	19	19	1	0
9	D	6	8	8	6	0
10	A	45	0	0	0	0
10	B	48	0	0	2	0
10	C	105	0	0	3	0
10	D	84	0	0	1	0
10	K	37	0	0	1	0
All	All	6119	27	5572	92	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 8.

All (92) 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)
2:B:7:ASN:HD21	7:B:501:NAG:H2	1.20	1.04
4:D:34:MET:HE1	4:D:96:CYS:HB2	1.57	0.84
1:A:78:ASN:OD1	6:E:1:NAG:C1	2.27	0.83
2:B:54:LYS:HB3	2:B:81:GLN:HG3	1.62	0.81
5:K:2:VAL:HG11	5:K:110:TYR:CE1	2.22	0.73
4:D:58:THR:H	9:D:301:GOL:H11	1.54	0.72
1:A:42:ARG:NH1	1:A:45:LYS:HD3	2.04	0.71
5:K:20:LEU:HG	5:K:83:MET:HE2	1.73	0.69
2:B:22:SER:O	2:B:23:ILE:HD13	1.94	0.67
3:C:197:VAL:HG22	3:C:216:ASN:OD1	1.94	0.67
2:B:7:ASN:ND2	7:B:501:NAG:H2	2.04	0.67
4:D:30:THR:HB	4:D:54:THR:HG22	1.76	0.67
3:C:138:VAL:HG22	3:C:154:TRP:CH2	2.31	0.65
3:C:65:ARG:HD2	3:C:81:PRO:O	2.00	0.62
4:D:12:VAL:O	4:D:115:VAL:HA	2.00	0.62
5:K:12:VAL:HG21	5:K:16:GLY:HA3	1.81	0.60
5:K:24:ALA:CB	5:K:29:ILE:HD11	2.31	0.60
5:K:18:LEU:HB2	5:K:83:MET:HE3	1.83	0.60
2:B:55:GLU:HB3	2:B:80:THR:OG1	2.01	0.60
3:C:132:LYS:N	3:C:132:LYS:HE2	2.17	0.60
3:C:138:VAL:HG13	3:C:185:LEU:HB3	1.85	0.58
2:B:7:ASN:HD21	7:B:501:NAG:C2	2.07	0.57
5:K:73:ASP:OD2	5:K:76:LYS:HD2	2.04	0.56
1:A:52:ASN:OD1	7:A:101:NAG:C1	2.53	0.56
4:D:58:THR:H	9:D:301:GOL:C1	2.18	0.56
5:K:39:GLN:HB2	5:K:45:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:LEU:O	3:C:189:LYS:HD3	2.06	0.55
3:C:52:ILE:HD13	3:C:58:LEU:HD23	1.87	0.55
10:C:301:HOH:O	4:D:44:GLY:HA3	2.06	0.55
1:A:25:ILE:HD11	6:E:1:NAG:H82	1.89	0.55
2:B:86:LYS:NZ	10:B:603:HOH:O	2.40	0.55
2:B:17:CYS:HB3	2:B:19:PHE:CE2	2.42	0.54
1:A:31:CYS:HA	2:B:32:CYS:O	2.07	0.54
4:D:30:THR:HA	4:D:53:PRO:HB2	1.89	0.54
1:A:42:ARG:HH12	1:A:45:LYS:HD3	1.72	0.54
5:K:2:VAL:HG11	5:K:110:TYR:CD1	2.43	0.54
5:K:12:VAL:CG2	5:K:16:GLY:HA3	2.38	0.53
4:D:12:VAL:HG11	4:D:86:LEU:HD22	1.90	0.53
3:C:98:TYR:HA	3:C:99:PRO:C	2.33	0.53
4:D:57:ARG:HA	9:D:301:GOL:H11	1.90	0.53
2:B:2:SER:O	2:B:30:GLY:HA3	2.09	0.53
4:D:34:MET:CE	4:D:96:CYS:HB2	2.34	0.52
5:K:31:ARG:HB2	5:K:32:TYR:CE1	2.43	0.52
4:D:3:GLN:NE2	10:D:405:HOH:O	2.41	0.52
4:D:182:LEU:C	4:D:182:LEU:HD23	2.34	0.52
3:C:58:LEU:HD21	3:C:66:PHE:O	2.10	0.51
5:K:91:THR:O	5:K:92:ALA:HB2	2.10	0.51
4:D:30:THR:O	4:D:54:THR:CG2	2.59	0.50
2:B:2:SER:HB3	2:B:31:TYR:HB2	1.93	0.50
4:D:57:ARG:HA	9:D:301:GOL:H32	1.94	0.49
2:B:24:ASN:OD1	7:B:500:NAG:C1	2.61	0.49
3:C:87:VAL:CG2	3:C:112:ILE:HG12	2.44	0.48
5:K:24:ALA:HB3	5:K:29:ILE:CD1	2.44	0.48
5:K:72:ARG:HB3	5:K:79:VAL:HG12	1.96	0.47
3:C:33:GLY:N	10:C:307:HOH:O	2.47	0.47
8:A:102:BTB:H82	10:B:615:HOH:O	2.14	0.47
4:D:57:ARG:HG2	9:D:301:GOL:H32	1.97	0.47
5:K:22:CYS:HB3	5:K:79:VAL:CG2	2.45	0.47
5:K:2:VAL:O	5:K:2:VAL:HG13	2.14	0.46
5:K:31:ARG:HB2	5:K:32:TYR:CD1	2.52	0.45
1:A:26:LEU:H	1:A:78:ASN:ND2	2.14	0.45
3:C:24:ARG:HA	3:C:73:THR:O	2.17	0.45
3:C:122:PHE:HB3	4:D:134:SER:HB2	1.99	0.45
3:C:214:SER:O	4:D:133:LYS:HD2	2.17	0.45
5:K:24:ALA:CB	5:K:29:ILE:CD1	2.94	0.45
5:K:20:LEU:CG	5:K:83:MET:HE2	2.45	0.44
4:D:33:TRP:HB2	4:D:99:ARG:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:308:HOH:O	4:D:213:LYS:NZ	2.50	0.43
1:A:10:CYS:HA	1:A:30:GLY:HA3	2.01	0.43
1:A:89:TYR:HD2	2:B:48:GLN:HG3	1.84	0.43
2:B:55:GLU:HB2	2:B:81:GLN:HG2	1.99	0.43
3:C:110:LEU:HD12	3:C:111:GLU:N	2.33	0.43
3:C:38:GLN:HG2	4:D:103:SER:CB	2.49	0.43
2:B:6:THR:HG21	2:B:29:ALA:HB3	2.01	0.43
5:K:34:MET:HG3	5:K:79:VAL:HG11	2.00	0.43
1:A:9:GLU:HG2	1:A:11:THR:HG23	2.00	0.43
3:C:113:LYS:HE3	5:K:59:PHE:CE2	2.53	0.42
2:B:46:LYS:HD2	2:B:46:LYS:HA	1.75	0.42
2:B:56:LEU:C	2:B:56:LEU:HD12	2.45	0.42
5:K:102:THR:HB	10:K:210:HOH:O	2.19	0.42
4:D:58:THR:N	9:D:301:GOL:H11	2.27	0.42
4:D:35:HIS:CE1	4:D:50:GLU:HB2	2.55	0.41
4:D:123:PRO:HB3	4:D:149:TYR:HB3	2.02	0.41
5:K:6:GLU:HA	5:K:21:SER:O	2.19	0.41
3:C:87:VAL:O	3:C:88:ALA:HB2	2.19	0.41
2:B:57:VAL:O	2:B:78:VAL:N	2.47	0.41
5:K:103:PHE:O	5:K:104:TYR:HB2	2.21	0.41
5:K:68:PHE:N	5:K:68:PHE:CD1	2.88	0.40
3:C:52:ILE:CD1	3:C:58:LEU:HD23	2.50	0.40
5:K:22:CYS:O	5:K:78:THR:HG23	2.22	0.40
3:C:11:LEU:N	3:C:11:LEU:HD23	2.37	0.40
4:D:40:ARG:O	4:D:43:GLN:HB2	2.21	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	85/92 (92%)	85 (100%)	0	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	104/111 (94%)	101 (97%)	3 (3%)	0	100	100
3	C	211/220 (96%)	205 (97%)	6 (3%)	0	100	100
4	D	214/225 (95%)	211 (99%)	2 (1%)	1 (0%)	24	31
5	K	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
All	All	731/775 (94%)	714 (98%)	16 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	137	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/83 (95%)	76 (96%)	3 (4%)	29	44
2	B	94/99 (95%)	93 (99%)	1 (1%)	65	81
3	C	189/194 (97%)	182 (96%)	7 (4%)	30	45
4	D	186/195 (95%)	178 (96%)	8 (4%)	26	39
5	K	95/103 (92%)	93 (98%)	2 (2%)	47	66
All	All	643/674 (95%)	622 (97%)	21 (3%)	33	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	CYS
1	A	67	ARG
1	A	76	VAL
2	B	46	LYS
3	C	22	SER
3	C	52	ILE
3	C	69	THR

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Mol	Chain	Res	Type
3	C	72	ARG
3	C	138	VAL
3	C	152	VAL
3	C	181	LEU
4	D	45	LEU
4	D	72	VAL
4	D	115	VAL
4	D	124	SER
4	D	139	THR
4	D	182	LEU
4	D	202	VAL
4	D	214	LYS
5	K	21	SER
5	K	102	THR

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

Mol	Chain	Res	Type
1	A	13	GLN
1	A	20	GLN
2	B	7	ASN
2	B	81	GLN
3	C	57	ASN
3	C	94	GLN
3	C	158	ASN
3	C	166	GLN
4	D	43	GLN

### 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	$\# Z  > 2$
6	NAG	E	1	6	14,14,15	0.97	1 (7%)	17,19,21	1.67	4 (23%)
6	NAG	E	2	6	14,14,15	0.71	0	17,19,21	1.17	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
6	NAG	E	1	6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1	NAG	O5-C1	-2.61	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1	NAG	C1-O5-C5	-4.11	106.68	112.19
6	E	2	NAG	C1-O5-C5	3.30	116.61	112.19
6	E	1	NAG	C2-N2-C7	2.94	126.84	122.90
6	E	1	NAG	O5-C1-C2	-2.33	107.69	111.29
6	E	1	NAG	O4-C4-C3	-2.23	105.12	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

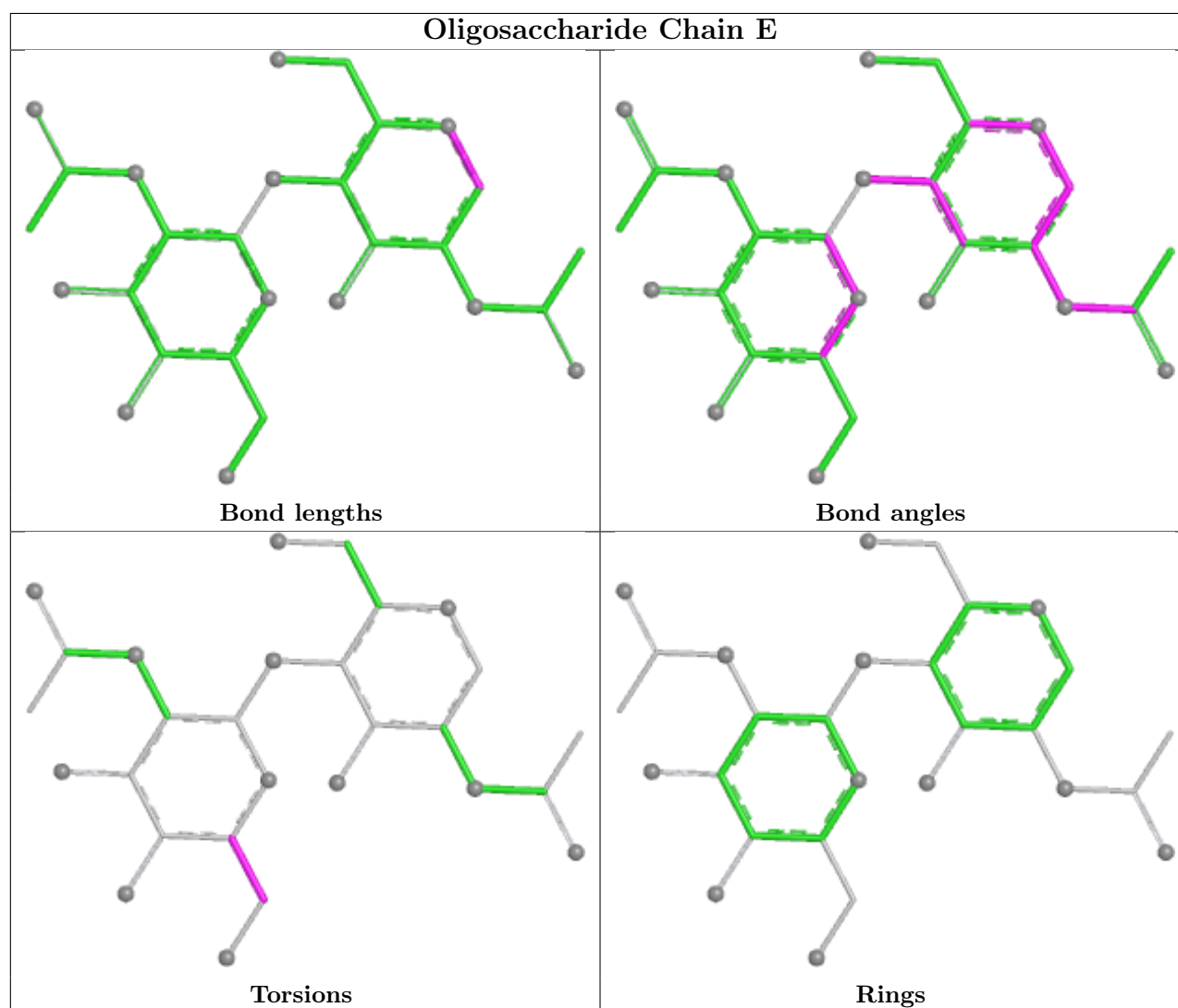
Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	101	-	14,14,15	0.71	0	17,19,21	2.35	6 (35%)
7	NAG	B	500	-	14,14,15	0.63	0	17,19,21	1.94	4 (23%)
8	BTB	A	102	-	13,13,13	0.99	1 (7%)	7,16,16	0.62	0
7	NAG	B	501	-	14,14,15	0.73	0	17,19,21	1.00	1 (5%)
9	GOL	D	301	-	5,5,5	0.33	0	5,5,5	0.56	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
7	NAG	A	101	-	-	3/6/23/26	0/1/1/1
7	NAG	B	500	-	-	2/6/23/26	0/1/1/1
8	BTB	A	102	-	-	7/21/21/21	-
7	NAG	B	501	-	-	0/6/23/26	0/1/1/1
9	GOL	D	301	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	102	BTB	C3-C2	2.13	1.55	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	101	NAG	O5-C1-C2	-5.35	103.02	111.29
7	B	500	NAG	C2-N2-C7	4.52	128.96	122.90
7	B	500	NAG	O5-C1-C2	-3.91	105.24	111.29
7	A	101	NAG	C2-N2-C7	3.75	127.93	122.90
7	A	101	NAG	C3-C4-C5	3.48	116.54	110.23
7	A	101	NAG	C4-C3-C2	3.44	116.05	111.02
7	A	101	NAG	C1-C2-N2	3.40	115.79	110.43
7	B	500	NAG	C1-C2-N2	2.80	114.85	110.43
7	B	500	NAG	C3-C4-C5	2.74	115.20	110.23
7	A	101	NAG	O3-C3-C2	-2.61	103.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	NAG	O5-C1-C2	-2.09	108.06	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	101	NAG	C1-C2-N2-C7
7	B	500	NAG	C1-C2-N2-C7
8	A	102	BTB	C1-C2-C4-O4
8	A	102	BTB	C3-C2-C4-O4
8	A	102	BTB	N-C2-C4-O4
7	A	101	NAG	O5-C5-C6-O6
7	B	500	NAG	O5-C5-C6-O6
7	A	101	NAG	C4-C5-C6-O6
8	A	102	BTB	N-C7-C8-O8
9	D	301	GOL	O1-C1-C2-C3
9	D	301	GOL	C1-C2-C3-O3
9	D	301	GOL	O1-C1-C2-O2
9	D	301	GOL	O2-C2-C3-O3
8	A	102	BTB	O1-C1-C2-C3
8	A	102	BTB	O1-C1-C2-N
8	A	102	BTB	C4-C2-N-C7

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	101	NAG	1	0
7	B	500	NAG	1	0
8	A	102	BTB	1	0
7	B	501	NAG	3	0
9	D	301	GOL	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	87/92 (94%)	0.06	1 (1%) 78 79	37, 47, 60, 82	0
2	B	106/111 (95%)	0.45	4 (3%) 44 46	39, 53, 65, 72	0
3	C	215/220 (97%)	0.09	5 (2%) 61 63	37, 48, 69, 99	0
4	D	216/225 (96%)	0.11	6 (2%) 55 57	38, 48, 64, 75	0
5	K	119/127 (93%)	0.28	3 (2%) 58 60	41, 51, 65, 77	0
All	All	743/775 (95%)	0.17	19 (2%) 57 59	37, 49, 67, 99	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	29	VAL	4.7
2	B	47	ILE	4.4
2	B	2	SER	3.8
4	D	134	SER	3.6
4	D	136	SER	3.3
3	C	218	GLY	3.1
4	D	133	LYS	2.8
5	K	29	ILE	2.6
4	D	137	GLY	2.6
3	C	70	GLY	2.4
5	K	9	GLY	2.4
5	K	3	GLN	2.4
2	B	74	TYR	2.3
4	D	132	SER	2.3
1	A	6	ASP	2.2
3	C	2	ILE	2.2
2	B	107	GLY	2.1
3	C	28	SER	2.1
4	D	218	LYS	2.1

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

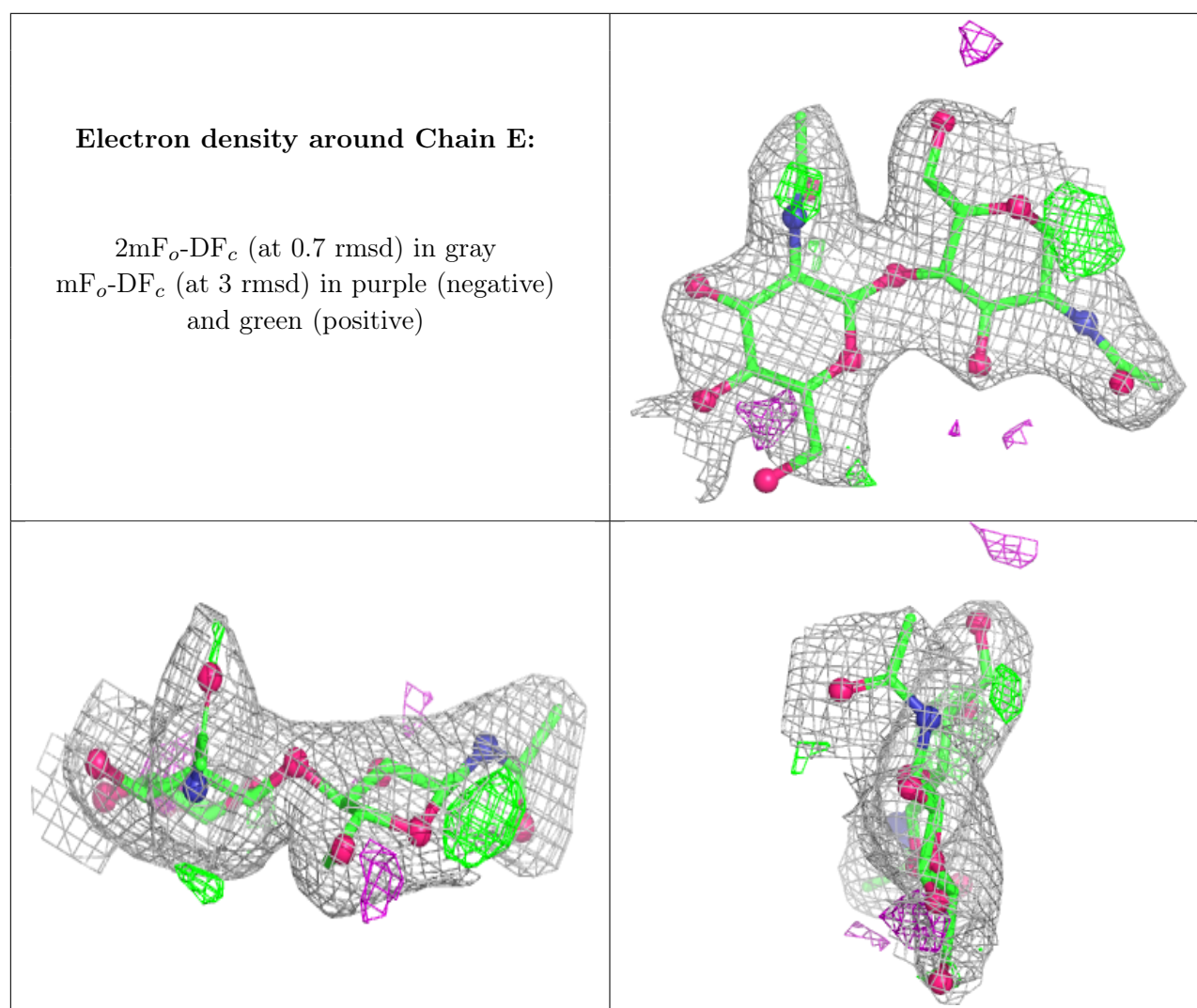
There are no non-standard protein/DNA/RNA residues in this entry.

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	E	1	14/15	-	-	45,52,60,68	0
6	NAG	E	2	14/15	-	-	69,76,85,88	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	B	501	14/15	0.54	0.21	86,94,99,100	0
7	NAG	B	500	14/15	0.62	0.18	74,84,89,89	0
9	GOL	D	301	6/6	0.72	0.14	62,75,86,93	0
7	NAG	A	101	14/15	0.75	0.18	66,71,74,76	0
8	BTB	A	102	14/14	0.85	0.14	47,59,65,71	33

## 6.5 Other polymers [i](#)

There are no such residues in this entry.