



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 02:43 AM UTC

PDB ID : 9EZA / pdb\_00009eza  
Title : Interleukin-31 Receptor D1D2 in complex with Nemolizumab derived scFv  
Authors : Bloch, Y.; Savvides, S.N.  
Deposited on : 2024-04-11  
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

---

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

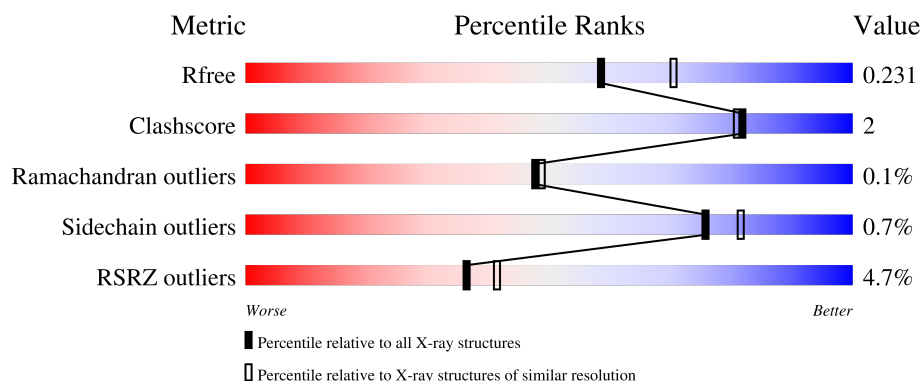
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	260	
1	C	260	
2	B	261	
2	D	261	
3	E	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13951 atoms, of which 6729 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 Nemolizumab scFv.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	236	Total	C	H	N	O	S	67	0	0
			3469	1115	1686	294	366	8			
1	C	234	Total	C	H	N	O	S	67	0	0
			3455	1111	1680	292	364	8			

- Molecule 2 is a protein called Interleukin-31 receptor subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	202	Total	C	H	N	O	S	55	2	0
			3294	1059	1633	282	310	10			
2	D	204	Total	C	H	N	O	S	55	0	0
			3295	1060	1631	281	313	10			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	225	GLY	-	expression tag	UNP Q8NI17
B	226	THR	-	expression tag	UNP Q8NI17
B	227	SER	-	expression tag	UNP Q8NI17
B	228	ASP	-	expression tag	UNP Q8NI17
B	229	GLU	-	expression tag	UNP Q8NI17
B	230	VAL	-	expression tag	UNP Q8NI17
B	231	ASP	-	expression tag	UNP Q8NI17
B	232	GLY	-	expression tag	UNP Q8NI17
B	233	GLY	-	expression tag	UNP Q8NI17
B	234	SER	-	expression tag	UNP Q8NI17
B	235	GLY	-	expression tag	UNP Q8NI17
B	236	GLY	-	expression tag	UNP Q8NI17
B	237	SER	-	expression tag	UNP Q8NI17
B	238	GLY	-	expression tag	UNP Q8NI17
B	239	LEU	-	expression tag	UNP Q8NI17
B	240	ASN	-	expression tag	UNP Q8NI17

*Continued on next page...*

*Continued from previous page...*

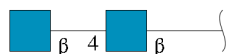
Chain	Residue	Modelled	Actual	Comment	Reference
B	241	ASP	-	expression tag	UNP Q8NI17
B	242	ILE	-	expression tag	UNP Q8NI17
B	243	PHE	-	expression tag	UNP Q8NI17
B	244	GLU	-	expression tag	UNP Q8NI17
B	245	ALA	-	expression tag	UNP Q8NI17
B	246	GLN	-	expression tag	UNP Q8NI17
B	247	LYS	-	expression tag	UNP Q8NI17
B	248	ILE	-	expression tag	UNP Q8NI17
B	249	GLU	-	expression tag	UNP Q8NI17
B	250	TRP	-	expression tag	UNP Q8NI17
B	251	HIS	-	expression tag	UNP Q8NI17
B	252	GLU	-	expression tag	UNP Q8NI17
B	253	GLY	-	expression tag	UNP Q8NI17
B	254	ARG	-	expression tag	UNP Q8NI17
B	255	THR	-	expression tag	UNP Q8NI17
B	256	LYS	-	expression tag	UNP Q8NI17
B	257	HIS	-	expression tag	UNP Q8NI17
B	258	HIS	-	expression tag	UNP Q8NI17
B	259	HIS	-	expression tag	UNP Q8NI17
B	260	HIS	-	expression tag	UNP Q8NI17
B	261	HIS	-	expression tag	UNP Q8NI17
B	262	HIS	-	expression tag	UNP Q8NI17
D	225	GLY	-	expression tag	UNP Q8NI17
D	226	THR	-	expression tag	UNP Q8NI17
D	227	SER	-	expression tag	UNP Q8NI17
D	228	ASP	-	expression tag	UNP Q8NI17
D	229	GLU	-	expression tag	UNP Q8NI17
D	230	VAL	-	expression tag	UNP Q8NI17
D	231	ASP	-	expression tag	UNP Q8NI17
D	232	GLY	-	expression tag	UNP Q8NI17
D	233	GLY	-	expression tag	UNP Q8NI17
D	234	SER	-	expression tag	UNP Q8NI17
D	235	GLY	-	expression tag	UNP Q8NI17
D	236	GLY	-	expression tag	UNP Q8NI17
D	237	SER	-	expression tag	UNP Q8NI17
D	238	GLY	-	expression tag	UNP Q8NI17
D	239	LEU	-	expression tag	UNP Q8NI17
D	240	ASN	-	expression tag	UNP Q8NI17
D	241	ASP	-	expression tag	UNP Q8NI17
D	242	ILE	-	expression tag	UNP Q8NI17
D	243	PHE	-	expression tag	UNP Q8NI17
D	244	GLU	-	expression tag	UNP Q8NI17

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	245	ALA	-	expression tag	UNP Q8NI17
D	246	GLN	-	expression tag	UNP Q8NI17
D	247	LYS	-	expression tag	UNP Q8NI17
D	248	ILE	-	expression tag	UNP Q8NI17
D	249	GLU	-	expression tag	UNP Q8NI17
D	250	TRP	-	expression tag	UNP Q8NI17
D	251	HIS	-	expression tag	UNP Q8NI17
D	252	GLU	-	expression tag	UNP Q8NI17
D	253	GLY	-	expression tag	UNP Q8NI17
D	254	ARG	-	expression tag	UNP Q8NI17
D	255	THR	-	expression tag	UNP Q8NI17
D	256	LYS	-	expression tag	UNP Q8NI17
D	257	HIS	-	expression tag	UNP Q8NI17
D	258	HIS	-	expression tag	UNP Q8NI17
D	259	HIS	-	expression tag	UNP Q8NI17
D	260	HIS	-	expression tag	UNP Q8NI17
D	261	HIS	-	expression tag	UNP Q8NI17
D	262	HIS	-	expression tag	UNP Q8NI17

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



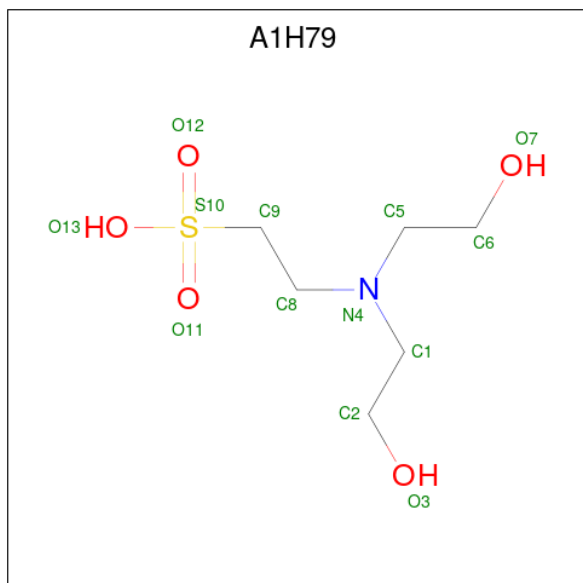
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	H	N	O	11	0	0
			55	16	27	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
4	B	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	6	0
			28	8	14	1	5		
4	D	1	Total	C	H	N	O	6	0
			28	8	14	1	5		

- Molecule 5 is BES buffer (CCD ID: A1H79) (formula:  $C_6H_{15}NO_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	S	
			29	6	16	1	5	1	
								3	0

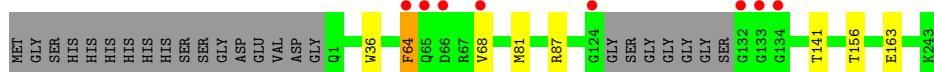
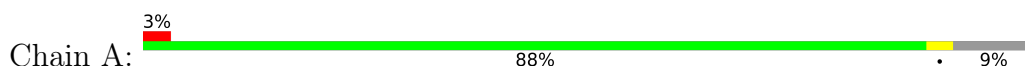
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	110	Total	O		
			110	110	0	0
6	B	12	Total	O		
			12	12	0	0
6	C	94	Total	O		
			94	94	0	0
6	D	26	Total	O		
			26	26	0	0

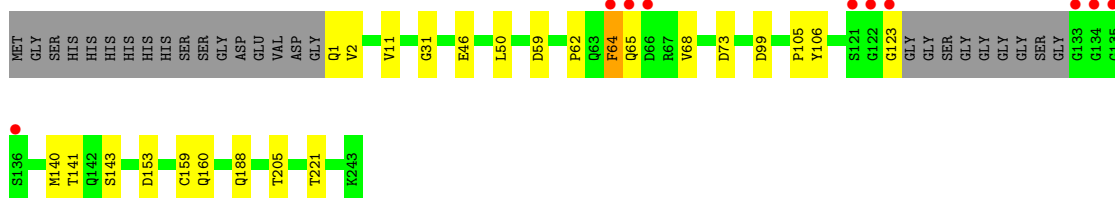
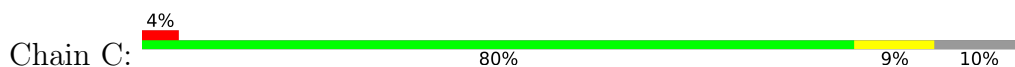
### 3 Residue-property plots [i](#)

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.

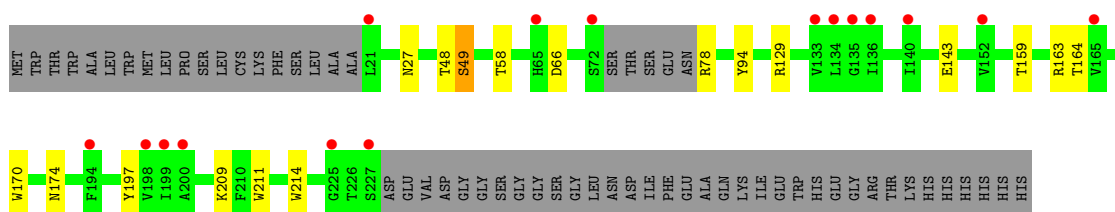
- Molecule 1: Nemolizumab scFv



- Molecule 1: Nemolizumab scFv



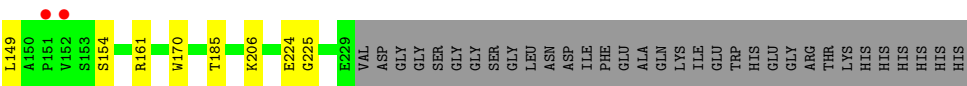
- Molecule 2: Interleukin-31 receptor subunit alpha



- Molecule 2: Interleukin-31 receptor subunit alpha







● Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1  
NAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.01Å 163.56Å 269.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.15 46.74 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.74-2.15) 99.5 (46.74-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.98 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.201 , 0.230 0.201 , 0.231	Depositor DCC
$R_{free}$ test set	2000 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: A1H79, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.62	0/1824	1.01	4/2476 (0.2%)
1	C	0.58	0/1816	1.00	9/2466 (0.4%)
2	B	0.51	0/1712	0.99	3/2320 (0.1%)
2	D	0.52	0/1706	1.00	1/2312 (0.0%)
All	All	0.56	0/7058	1.00	17/9574 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	209	LYS	N-CA-CB	-7.70	97.85	110.40
1	A	64	PHE	CA-CB-CG	7.56	121.36	113.80
1	C	141	THR	CA-CB-OG1	-7.11	98.94	109.60
1	C	221	THR	CA-CB-OG1	-6.63	99.65	109.60
1	C	64	PHE	CB-CA-C	-6.49	98.58	109.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	ARG	Sidechain

## 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	1783	1686	1685	3	0
1	C	1775	1680	1679	9	0
2	B	1661	1633	1621	12	0
2	D	1664	1631	1623	11	0
3	E	28	27	25	0	0
4	B	28	28	26	0	0
4	D	28	28	26	0	0
5	D	13	16	0	0	0
6	A	110	0	0	0	0
6	B	12	0	0	0	0
6	C	94	0	0	0	0
6	D	26	0	0	0	0
All	All	7222	6729	6685	34	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 2.

The worst 5 of 34 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:27:ASN:O	2:B:78:ARG:NH2	2.20	0.75
2:B:129:ARG:NH2	2:B:143:GLU:OE1	2.22	0.72
1:A:64:PHE:HB3	1:A:68:VAL:HG23	1.73	0.71
1:C:62:PRO:HA	1:C:65:GLN:HB2	1.75	0.68
1:C:64:PHE:HB3	1:C:68:VAL:HG23	1.79	0.63

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	232/260 (89%)	224 (97%)	8 (3%)	0	100	100
1	C	230/260 (88%)	223 (97%)	7 (3%)	0	100	100
2	B	200/261 (77%)	189 (94%)	10 (5%)	1 (0%)	24	19
2	D	200/261 (77%)	189 (94%)	11 (6%)	0	100	100
All	All	862/1042 (83%)	825 (96%)	36 (4%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	49	SER

### 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	192/208 (92%)	192 (100%)	0	100	100
1	C	192/208 (92%)	190 (99%)	2 (1%)	68	74
2	B	186/234 (80%)	186 (100%)	0	100	100
2	D	185/234 (79%)	182 (98%)	3 (2%)	55	61
All	All	755/884 (85%)	750 (99%)	5 (1%)	76	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	46	GLU
1	C	143	SER
2	D	81	CYS
2	D	154	SER
2	D	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
2	B	174	ASN
1	C	39	GLN
1	C	43	GLN
2	D	174	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	$\# Z  > 2$
3	NAG	E	1	3,2	14,14,15	0.24	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.40	0	17,19,21	1.19	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	E	2	NAG	C1-C2-N2	2.88	114.97	110.43
3	E	1	NAG	C1-C2-N2	2.10	113.75	110.43

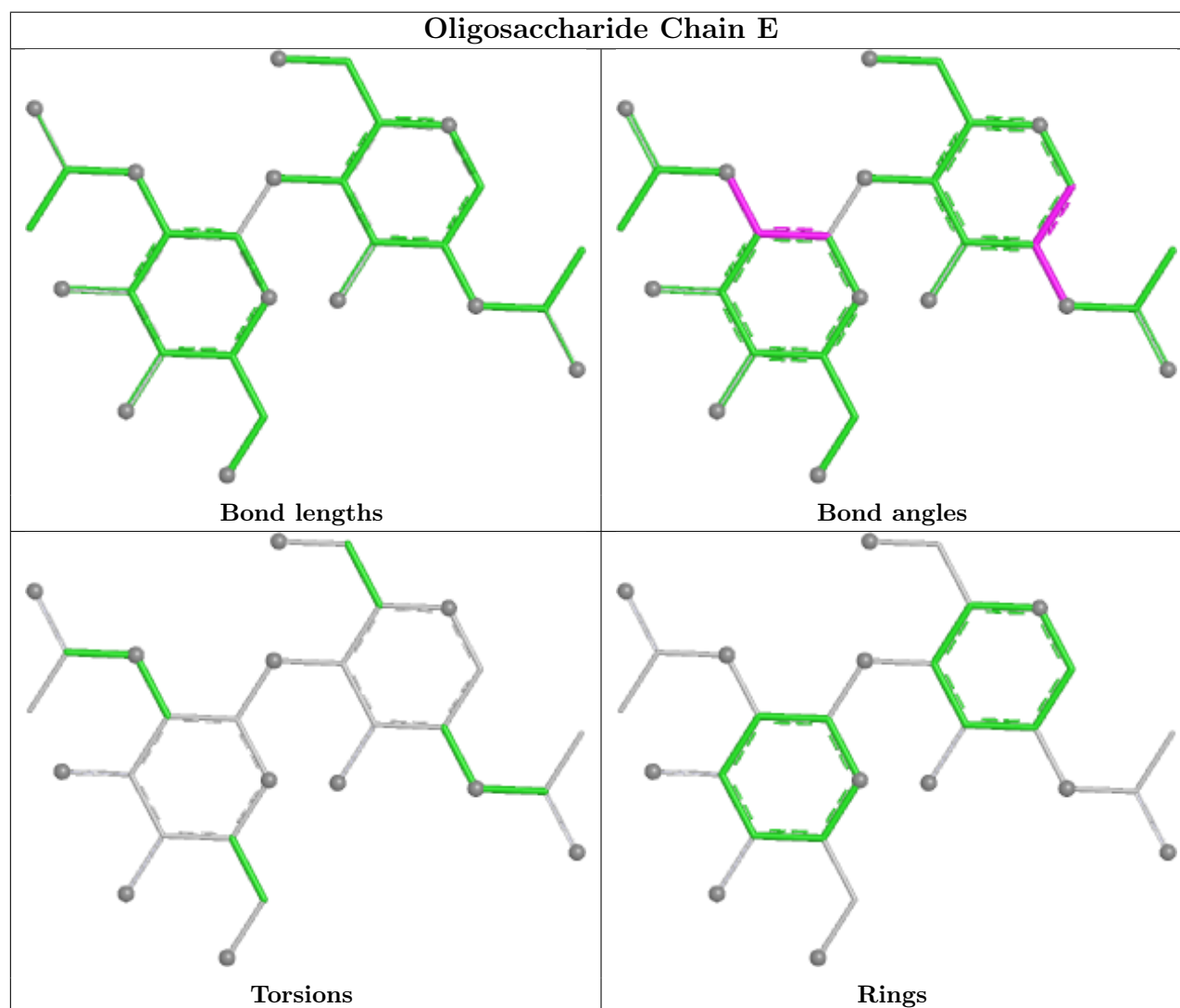
There are no chirality outliers.

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

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
5	A1H79	D	303	-	12,12,12	0.97	0	14,15,15	0.73	0
4	NAG	B	301	2	14,14,15	0.28	0	17,19,21	0.94	1 (5%)
4	NAG	D	301	2	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	D	302	2	14,14,15	0.38	0	17,19,21	1.09	3 (17%)
4	NAG	B	302	2	14,14,15	0.32	0	17,19,21	1.26	2 (11%)

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
5	A1H79	D	303	-	-	6/12/12/12	-
4	NAG	B	301	2	-	0/6/23/26	0/1/1/1
4	NAG	D	301	2	-	4/6/23/26	0/1/1/1
4	NAG	D	302	2	-	2/6/23/26	0/1/1/1
4	NAG	B	302	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	302	NAG	C2-N2-C7	3.61	127.74	122.90
4	D	302	NAG	C2-N2-C7	2.76	126.60	122.90
4	B	301	NAG	C1-C2-N2	2.72	114.73	110.43
4	B	302	NAG	C4-C3-C2	2.25	114.31	111.02
4	D	302	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.



5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	303	A1H79	C8-C9-S10-O11
5	D	303	A1H79	C8-C9-S10-O12
5	D	303	A1H79	C8-C9-S10-O13
4	D	301	NAG	C8-C7-N2-C2
4	D	301	NAG	O7-C7-N2-C2

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	236/260 (90%)	-0.42	8 (3%)	48	52	35, 46, 74, 103	0
1	C	234/260 (90%)	-0.31	10 (4%)	40	45	39, 52, 79, 97	0
2	B	202/261 (77%)	0.57	16 (7%)	18	21	33, 86, 141, 161	1 (0%)
2	D	204/261 (78%)	0.34	7 (3%)	48	52	45, 72, 113, 143	0
All	All	876/1042 (84%)	0.01	41 (4%)	36	41	33, 58, 116, 161	1 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	198	VAL	4.4
1	A	132	GLY	4.1
2	B	194	PHE	3.9
2	B	65[A]	HIS	3.7
2	B	225	GLY	3.7

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

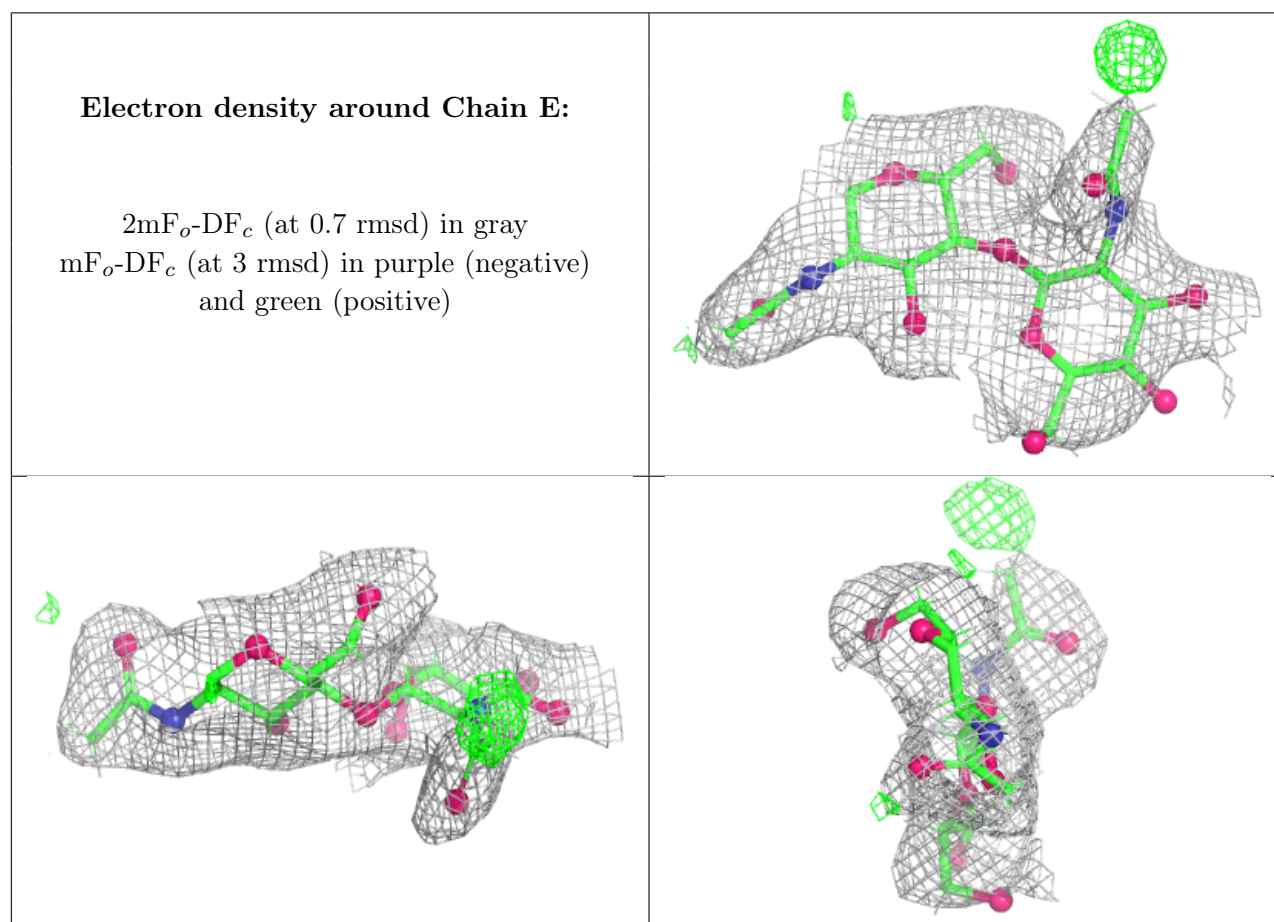
There are no non-standard protein/DNA/RNA residues in this entry.

### 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(Å <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.72	0.14	75,111,120,137	6
3	NAG	E	1	14/15	0.94	0.07	50,59,65,77	5

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(Å <sup>2</sup> )	Q<0.9
4	NAG	D	302	14/15	0.79	0.13	70,93,113,117	6
4	NAG	B	302	14/15	0.88	0.12	67,78,84,85	6
4	NAG	D	301	14/15	0.90	0.11	63,79,85,87	6
4	NAG	B	301	14/15	0.92	0.10	44,55,66,74	6
5	A1H79	D	303	13/13	0.92	0.12	70,96,104,113	3

## 6.5 Other polymers [i](#)

There are no such residues in this entry.