W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2025 – 12:16 pm GMT

PDB ID	:	9ETH
Title	:	Complex structure of IL-36R D1-D2 domain with 36R-P192 and BI655130 Fab
Authors	:	Scheufler, C.; Wirth, E.; Lehmann, S.
Deposited on	:	2024-03-26
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.30 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.
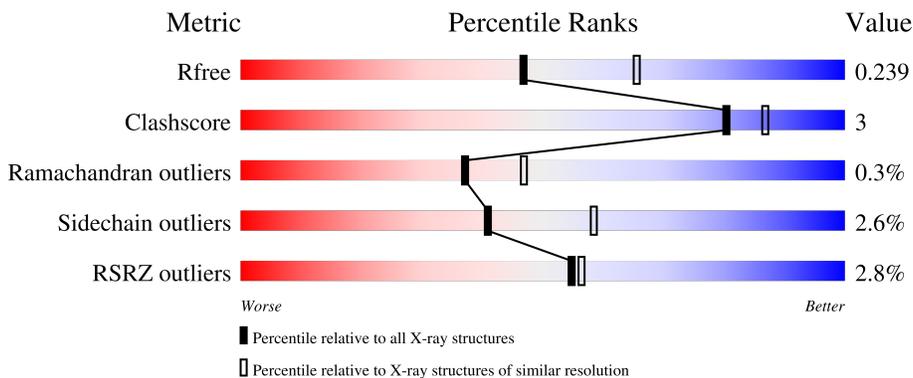
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	221	
2	L	215	
3	P	16	
4	R	207	
5	B	2	
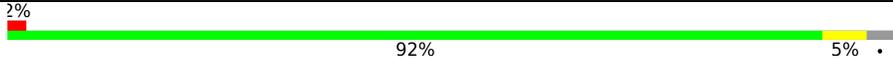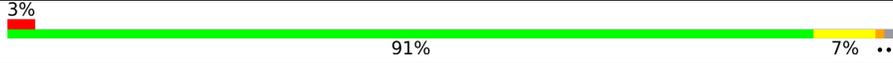
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Mol	Chain	Length	Quality of chain
6	C	6	33% 33% 33%
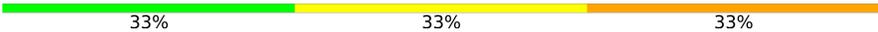
2 Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 5229 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 BI00655130 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total 1620	C 1030	N 268	O 315	S 7	0	0	0

- Molecule 2 is a protein called BI00655130 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total 1623	C 1020	N 277	O 321	S 5	0	1	0

- Molecule 3 is a protein called ACE-PHE-VAL-GLU-5CW-3PN-TRP-ASP-TYR-VAL-CHG-6G5-SER-GLU-CYS-NH2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	16	Total 145	C 99	Cl 2	N 20	O 23	S 1	0	0	1

- Molecule 4 is a protein called Interleukin-1 receptor-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	197	Total 1524	C 972	N 258	O 283	S 11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	221	HIS	-	expression tag	UNP Q9HB29
R	222	HIS	-	expression tag	UNP Q9HB29
R	223	HIS	-	expression tag	UNP Q9HB29
R	224	HIS	-	expression tag	UNP Q9HB29
R	225	HIS	-	expression tag	UNP Q9HB29
R	226	HIS	-	expression tag	UNP Q9HB29

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.


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

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alp ha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
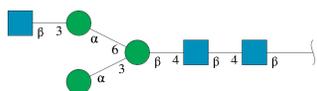
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	C	6	Total 75	C 42	N 3	O 30	0	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
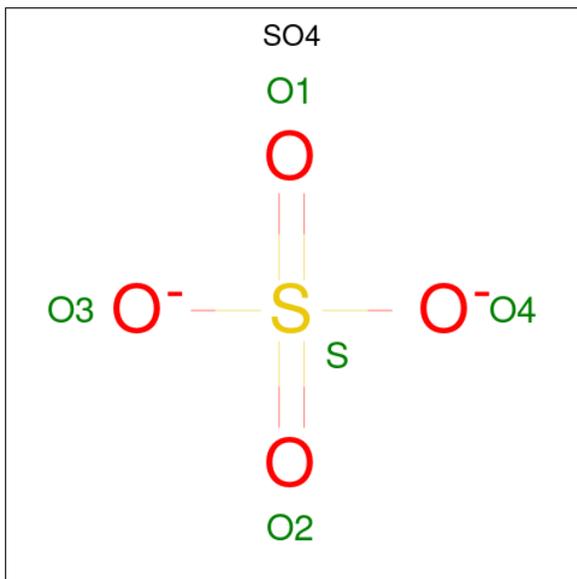
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total 5	O 4	S 1			0	0
7	H	1	Total 5	O 4	S 1			0	0
7	L	1	Total 5	O 4	S 1			0	0
7	L	1	Total 5	O 4	S 1			0	0
7	L	1	Total 5	O 4	S 1			0	0
7	L	1	Total 5	O 4	S 1			0	0
7	R	1	Total 5	O 4	S 1			0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total 1	Na 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
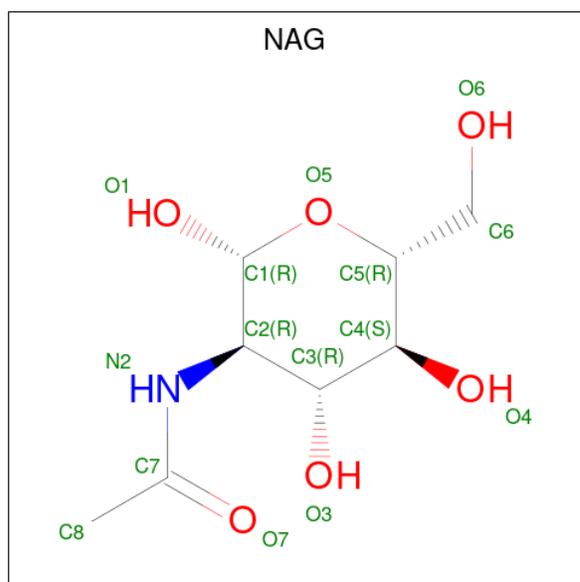
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	R	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
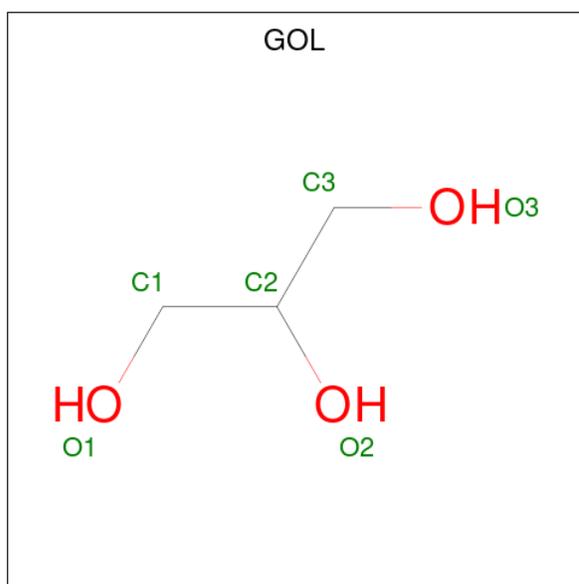
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	R	1	Total 6	C 3	O 3	0	0

- Molecule 11 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	59	Total 59	O 59	0	0
11	L	50	Total 50	O 50	0	0
11	P	5	Total 5	O 5	0	0
11	R	39	Total 39	O 39	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: BI00655130 Fab heavy chain
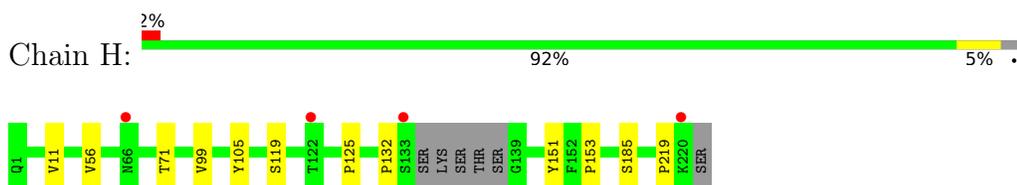
Chain H:

- Molecule 2: BI00655130 Fab light chain

Chain L:
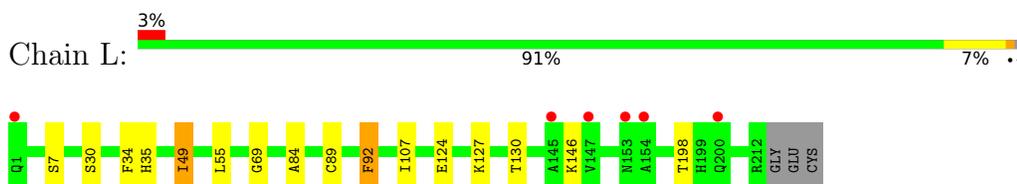
- Molecule 3: ACE-PHE-VAL-GLU-5CW-3PN-TRP-ASP-TYR-VAL-CHG-6G5-SER-GLU-CYS-NH2

Chain P:
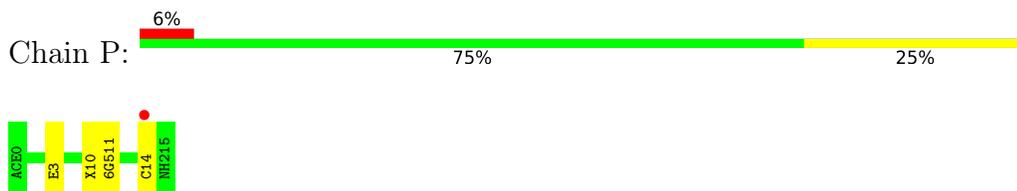
- Molecule 4: Interleukin-1 receptor-like 2

Chain R:
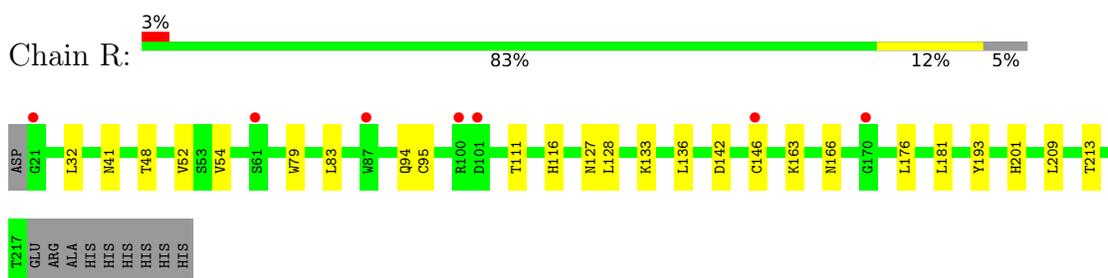
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[al pha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

33%   33%   33%
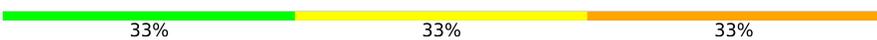
NAG1
NAG2
BMA3
MAN4
MAG5
MAN6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	54.64Å 175.35Å 191.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 2.30 32.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.8 (32.29-2.30) 88.8 (32.29-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.212 , 0.237 0.213 , 0.239	Depositor DCC
R_{free} test set	1781 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5229	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1H6Z, NA, 5CW, GOL, BMA, MAN, ACE, 6G5, SO4, NH2, NAG, CHG

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	H	0.42	0/1663	0.59	0/2272
2	L	0.35	0/1663	0.56	0/2265
3	P	0.35	0/91	0.55	0/121
4	R	0.39	0/1563	0.59	0/2129
All	All	0.38	0/4980	0.58	0/6787

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 ⓘ

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	H	1620	0	1568	5	0
2	L	1623	0	1546	7	0
3	P	145	0	94	1	0
4	R	1524	0	1442	12	0
5	B	28	0	25	0	0
6	C	75	0	64	3	0
7	H	15	0	0	0	0
7	L	20	0	0	0	0
7	R	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1	0	0	0	0
9	R	14	0	13	0	0
10	R	6	0	8	2	0
11	H	59	0	0	0	0
11	L	50	0	0	0	0
11	P	5	0	0	0	0
11	R	39	0	0	0	0
All	All	5229	0	4760	25	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.

The worst 5 of 25 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:H:11:VAL:HB	1:H:153:PRO:HG3	1.57	0.83
1:H:132:PRO:HG2	1:H:219:PRO:HB3	1.85	0.59
4:R:79:TRP:HE1	10:R:303:GOL:H11	1.69	0.57
1:H:125:PRO:HB3	1:H:151:TYR:HB3	1.90	0.53
3:P:3:GLU:HB2	3:P:10:CHG:H1	1.90	0.51

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	H	211/221 (96%)	207 (98%)	3 (1%)	1 (0%)	25	32
2	L	211/215 (98%)	207 (98%)	3 (1%)	1 (0%)	25	32
3	P	10/16 (62%)	10 (100%)	0	0	100	100
4	R	195/207 (94%)	182 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	627/659 (95%)	606 (97%)	19 (3%)	2 (0%)	37	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	69	GLY
1	H	56	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	H	181/191 (95%)	178 (98%)	3 (2%)	56	72
2	L	178/188 (95%)	173 (97%)	5 (3%)	38	55
3	P	10/10 (100%)	9 (90%)	1 (10%)	6	8
4	R	167/188 (89%)	162 (97%)	5 (3%)	36	52
All	All	536/577 (93%)	522 (97%)	14 (3%)	41	58

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	130	THR
3	P	14	CYS
4	R	213	THR
4	R	146	CYS
4	R	166	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	43	GLN
2	L	148	GLN
4	R	94	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	5CW	P	4	3	14,16,17	0.78	0	14,22,24	0.64	0
3	6G5	P	11	3	14,16,17	0.99	1 (7%)	12,22,24	1.19	1 (8%)
3	CHG	P	10	3	9,10,11	0.46	0	7,12,14	0.77	0
3	A1H6Z	P	5	3	11,12,13	0.33	0	12,15,17	0.26	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
3	5CW	P	4	3	-	0/4/6/8	0/2/2/2
3	6G5	P	11	3	-	0/4/6/8	0/2/2/2
3	CHG	P	10	3	-	1/5/14/16	0/1/1/1
3	A1H6Z	P	5	3	-	0/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	11	6G5	C8-C6	2.08	1.44	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	11	6G5	CB-C8-C7	-2.91	124.38	127.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	10	CHG	O-C-CA-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	10	CHG	1	0

5.5 Carbohydrates (i)

8 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	$\#|Z| > 2$
5	NAG	B	1	5,4	14,14,15	0.27	0	17,19,21	0.56	0
5	NAG	B	2	5	14,14,15	0.30	0	17,19,21	0.49	0
6	NAG	C	1	6,4	14,14,15	0.25	0	17,19,21	0.87	1 (5%)
6	NAG	C	2	6	14,14,15	0.26	0	17,19,21	0.49	0
6	BMA	C	3	6	11,11,12	0.24	0	15,15,17	0.49	0
6	MAN	C	4	6	11,11,12	0.29	0	15,15,17	0.72	1 (6%)
6	NAG	C	5	6	14,14,15	0.55	0	17,19,21	1.53	3 (17%)
6	MAN	C	6	6	11,11,12	0.26	0	15,15,17	0.65	1 (6%)

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	NAG	B	1	5,4	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	0/2/19/22	0/1/1/1
6	MAN	C	4	6	-	0/2/19/22	0/1/1/1
6	NAG	C	5	6	-	4/6/23/26	0/1/1/1
6	MAN	C	6	6	-	0/2/19/22	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(^{o})	Ideal(^{o})
6	C	5	NAG	C1-O5-C5	4.39	118.14	112.19
6	C	5	NAG	C2-N2-C7	3.17	127.42	122.90
6	C	5	NAG	C4-C3-C2	2.52	114.71	111.02
6	C	4	MAN	C1-O5-C5	2.50	115.57	112.19
6	C	6	MAN	C1-O5-C5	2.27	115.27	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	C	5	NAG	C8-C7-N2-C2
6	C	5	NAG	O7-C7-N2-C2
6	C	5	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	1	0
6	C	5	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.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings
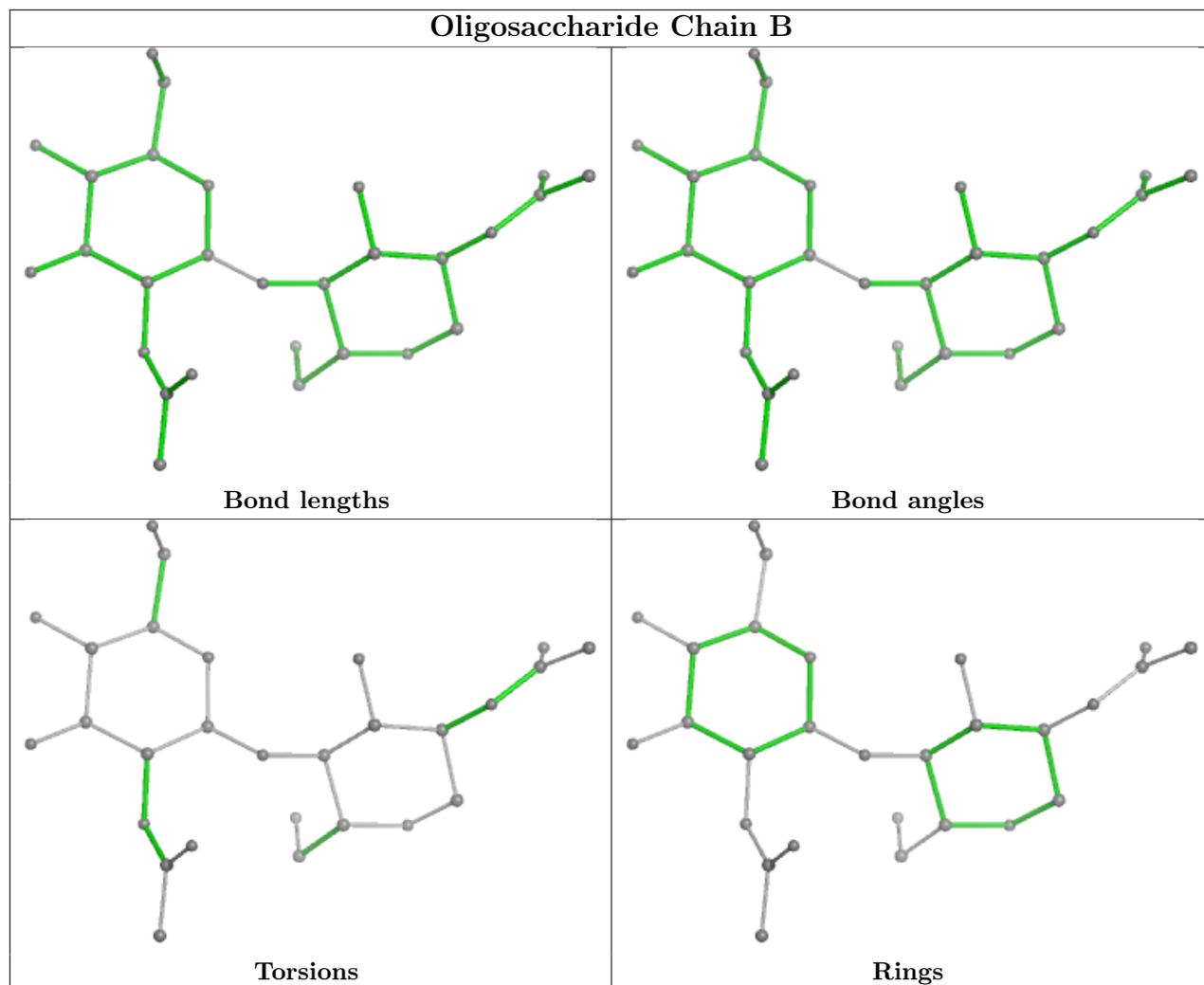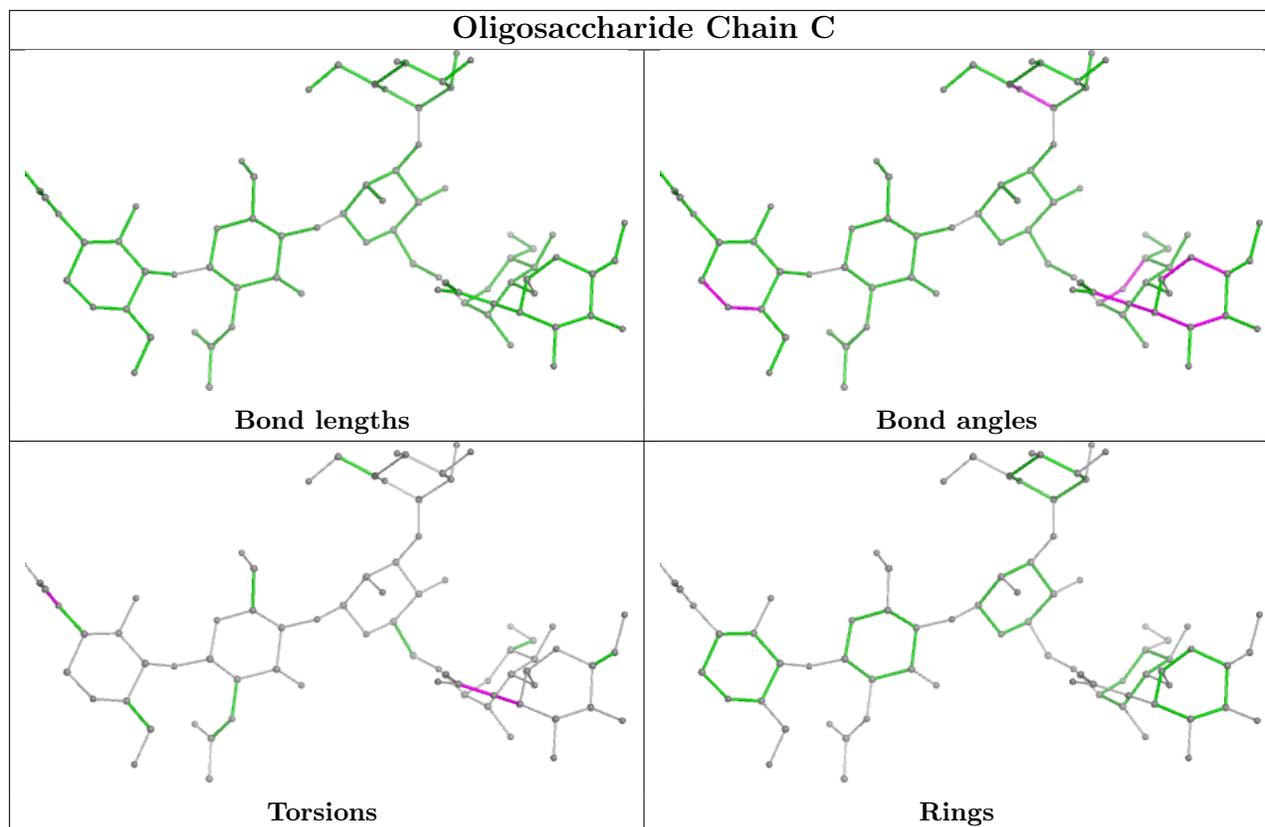
5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#|Z| > 2$
7	SO4	L	301	-	4,4,4	0.18	0	6,6,6	0.31	0
7	SO4	H	301	8	4,4,4	0.15	0	6,6,6	0.41	0
7	SO4	L	303	-	4,4,4	0.21	0	6,6,6	0.17	0
9	NAG	R	301	4	14,14,15	0.27	0	17,19,21	0.64	0
7	SO4	H	302	-	4,4,4	0.18	0	6,6,6	0.21	0
7	SO4	L	304	-	4,4,4	0.16	0	6,6,6	0.16	0
7	SO4	L	302	-	4,4,4	0.18	0	6,6,6	0.19	0
10	GOL	R	303	-	5,5,5	0.06	0	5,5,5	0.38	0
7	SO4	H	303	-	4,4,4	0.17	0	6,6,6	0.36	0
7	SO4	R	302	-	4,4,4	0.16	0	6,6,6	0.17	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
9	NAG	R	301	4	-	0/6/23/26	0/1/1/1
10	GOL	R	303	-	-	0/4/4/4	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	303	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	H	215/221 (97%)	0.09	4 (1%)	66	67	32, 52, 77, 89	0
2	L	212/215 (98%)	0.26	6 (2%)	55	56	39, 64, 81, 91	1 (0%)
3	P	10/16 (62%)	0.37	1 (10%)	14	15	45, 55, 68, 70	0
4	R	197/207 (95%)	0.38	7 (3%)	46	48	44, 61, 77, 85	0
All	All	634/659 (96%)	0.24	18 (2%)	55	56	32, 59, 79, 91	1 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	101	ASP	5.1
2	L	145	ALA	3.6
4	R	100	ARG	3.2
1	H	122	THR	3.2
4	R	61	SER	2.9

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

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
3	6G5	P	11	15/16	0.88	0.11	48,51,54,58	0
3	A1H6Z	P	5	12/13	0.93	0.09	46,48,50,50	0
3	CHG	P	10	10/11	0.96	0.08	42,43,46,46	0
3	5CW	P	4	15/16	0.97	0.06	44,44,46,47	0

6.3 Carbohydrates ⓘ

SUGAR-RSR INFOmissingINFO

6.4 Ligands ⓘ

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
7	SO4	L	304	5/5	0.66	0.11	167,167,167,167	0
7	SO4	L	301	5/5	0.67	0.10	114,114,114,114	0
9	NAG	R	301	14/15	0.68	0.16	93,94,95,95	0
7	SO4	L	302	5/5	0.73	0.13	126,127,127,127	0
7	SO4	R	302	5/5	0.78	0.08	125,125,125,125	0
7	SO4	L	303	5/5	0.79	0.12	102,102,102,102	0
10	GOL	R	303	6/6	0.83	0.15	74,75,75,75	0
7	SO4	H	303	5/5	0.85	0.08	127,127,127,127	0
7	SO4	H	302	5/5	0.86	0.11	102,102,102,103	0
8	NA	H	304	1/1	0.95	0.20	85,85,85,85	1
7	SO4	H	301	5/5	0.99	0.03	41,42,42,42	5

6.5 Other polymers ⓘ

There are no such residues in this entry.