Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 02:04 PM EDT

PDB ID	:	6DF3
Title	:	Crystal structure of ternary complex of IL-24 with soluble receptors IL-22RA and IL-20RB
Authors	:	Lubkowski, J.; Wlodawer, A.
Deposited on	:	2018-05-14
Resolution	:	2.15 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:

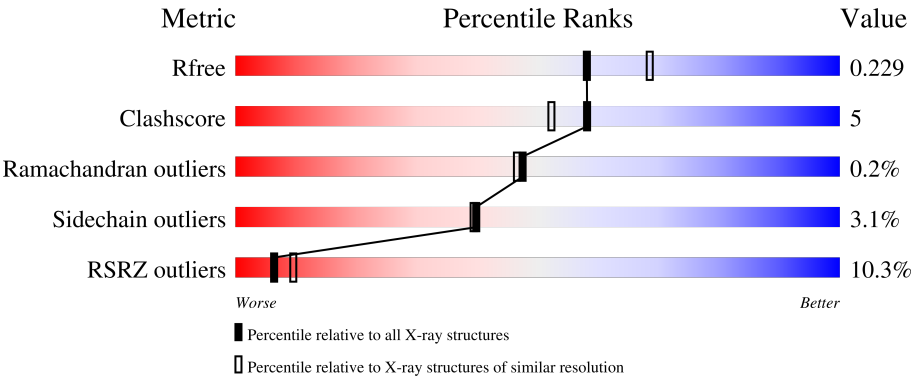
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	L	206	11% 83% 11%
2	C	155	% 83% 17%
3	H	190	17% 90% 9%
4	A	2	50% 50%

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
6	GOL	C	302	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4529 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 Interleukin-22 receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	199	Total	C	N	O	S	0	0	0
			1610	1024	277	299	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	229	GLY	-	expression tag	UNP Q8N6P7

- Molecule 2 is a protein called Interleukin-24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	155	Total	C	N	O	S	0	0	0
			1283	828	222	228	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	85	GLN	ASN	engineered mutation	UNP Q13007
C	99	GLN	ASN	engineered mutation	UNP Q13007
C	124	HIS	TYR	conflict	UNP Q13007
C	126	GLN	ASN	engineered mutation	UNP Q13007

- Molecule 3 is a protein called Interleukin-20 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	190	Total	C	N	O	S	0	0	0
			1502	962	247	284	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	134	GLN	ASN	engineered mutation	UNP Q6UXL0

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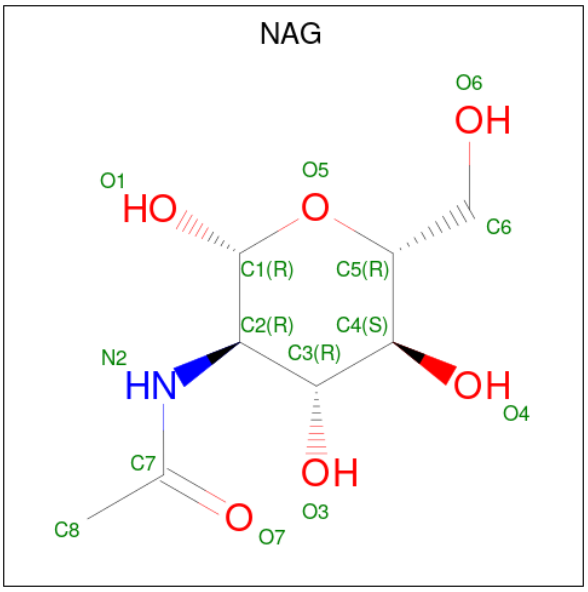
Chain	Residue	Modelled	Actual	Comment	Reference
H	206	GLU	GLN	conflict	UNP Q6UXL0

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

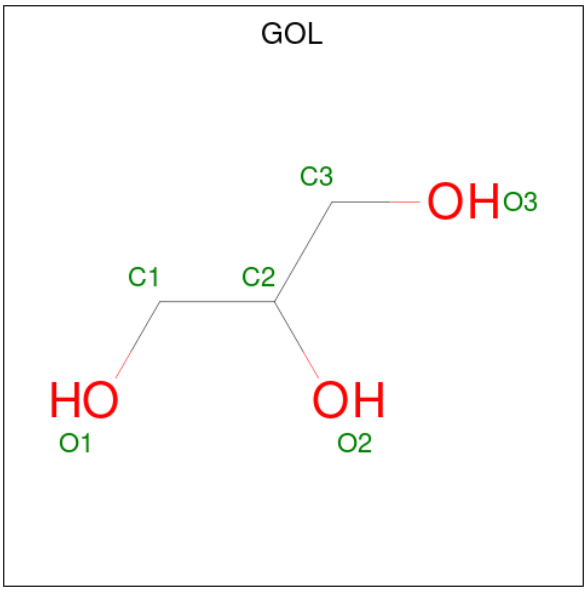
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	A	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

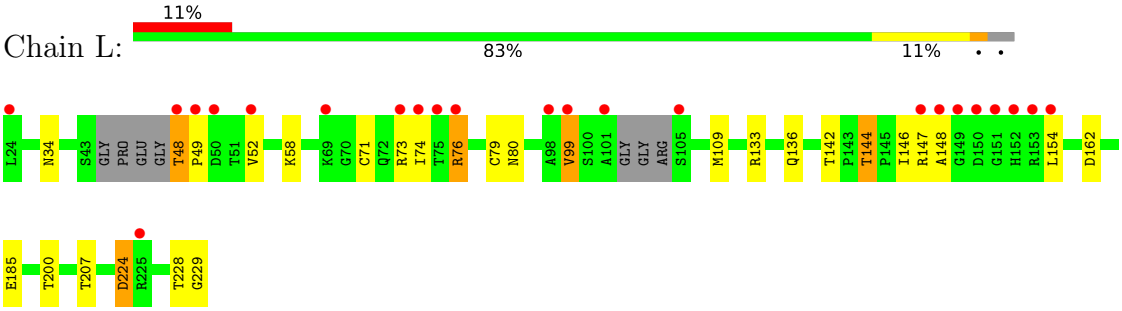
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	14	Total O 14 14	0	0
7	C	28	Total O 28 28	0	0
7	H	38	Total O 38 38	0	0

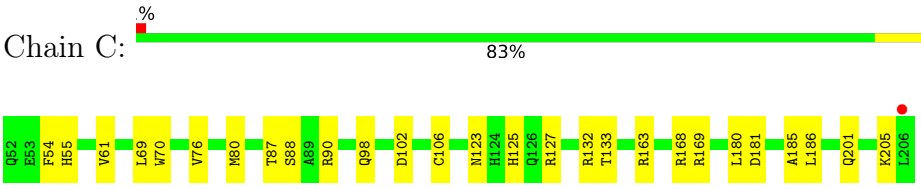
3 Residue-property plots (i)

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.

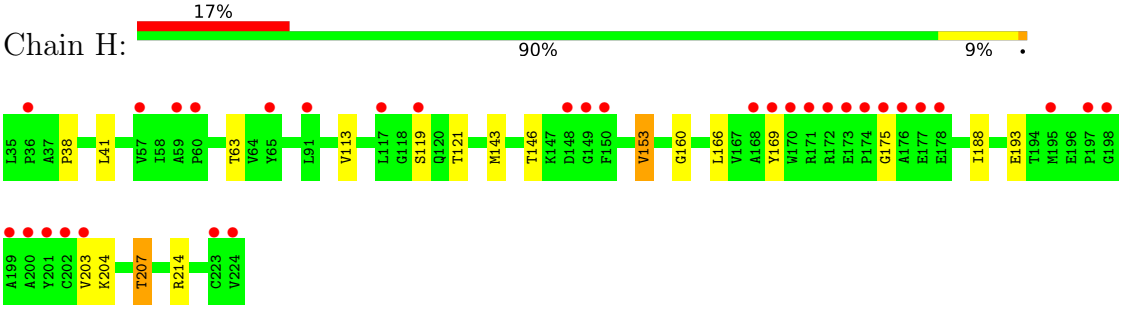
• Molecule 1: Interleukin-22 receptor subunit alpha-1



• Molecule 2: Interleukin-24



• Molecule 3: Interleukin-20 receptor subunit beta



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	77.70Å 77.70Å 124.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 34.75 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.15) 99.7 (34.75-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.182 , 0.225 0.190 , 0.229	Depositor DCC
R_{free} test set	1978 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å^2)	76.0	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.*

[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: NAG, GOL

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	L	0.94	0/1649	1.01	3/2238 (0.1%)
2	C	1.01	0/1311	1.04	7/1771 (0.4%)
3	H	0.93	0/1545	0.96	1/2109 (0.0%)
All	All	0.96	0/4505	1.00	11/6118 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	186	LEU	CA-CB-CG	9.74	137.69	115.30
2	C	168	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	C	102	ASP	CB-CG-OD1	6.88	124.49	118.30
2	C	168	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	L	224	ASP	CB-CG-OD1	5.64	123.38	118.30
2	C	163	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	L	76	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	H	214	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	C	106	CYS	CA-CB-SG	-5.38	104.32	114.00
1	L	73	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	C	90	ARG	NE-CZ-NH1	5.11	122.86	120.30

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	L	1610	0	1581	18	0
2	C	1283	0	1289	14	0
3	H	1502	0	1456	10	0
4	A	28	0	25	1	0
5	L	14	0	13	0	0
6	C	12	0	16	6	0
7	C	28	0	0	1	0
7	H	38	0	0	4	0
7	L	14	0	0	1	0
All	All	4529	0	4380	41	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 5.

All (41) 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)
3:H:146:THR:HG23	3:H:153:VAL:HG13	1.42	0.98
1:L:144:THR:HG22	1:L:146:ILE:H	1.47	0.78
2:C:201:GLN:OE1	6:C:302:GOL:O2	2.13	0.66
3:H:160:GLY:HA2	7:H:328:HOH:O	1.95	0.66
2:C:69:LEU:HB2	6:C:302:GOL:H11	1.80	0.64
1:L:80:ASN:HD22	4:A:1:NAG:H83	1.63	0.63
1:L:144:THR:HB	1:L:154:LEU:O	1.98	0.63
2:C:123:ASN:O	2:C:127:ARG:HG3	2.04	0.57
3:H:41:LEU:HD21	3:H:113:VAL:HG12	1.85	0.56
2:C:98:GLN:O	2:C:169:ARG:NH2	2.39	0.56
1:L:148:ALA:HB2	1:L:154:LEU:HD21	1.88	0.56
1:L:34:ASN:HD21	1:L:142:THR:HG21	1.71	0.55
1:L:71:CYS:HG	1:L:79:CYS:HG	1.52	0.54
1:L:200:THR:HG23	7:L:401:HOH:O	2.07	0.54
1:L:162:ASP:OD2	1:L:207:THR:OG1	2.16	0.54
1:L:133:ARG:NH2	1:L:224:ASP:OD2	2.41	0.53
2:C:55:HIS:HB2	2:C:205:LYS:HE3	1.90	0.53
3:H:207:THR:HG21	7:H:306:HOH:O	2.10	0.50
2:C:76:VAL:HG11	2:C:133:THR:HA	1.92	0.50
1:L:58:LYS:NZ	2:C:87:THR:OG1	2.45	0.50
1:L:74:ILE:HD12	1:L:76:ARG:HG2	1.93	0.49
3:H:188:ILE:N	7:H:301:HOH:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:169:TYR:HB3	3:H:203:VAL:HG12	1.96	0.48
3:H:143:MET:HE1	3:H:204:LYS:HA	1.96	0.47
2:C:54:PHE:HB2	2:C:61:VAL:HB	1.96	0.47
1:L:136:GLN:NE2	1:L:185:GLU:OE2	2.50	0.45
2:C:70:TRP:NE1	6:C:302:GOL:O1	2.50	0.45
1:L:48:THR:HG22	1:L:49:PRO:HD2	1.99	0.44
1:L:52:VAL:HG22	1:L:99:VAL:HG13	2.00	0.44
3:H:38:PRO:HG2	3:H:113:VAL:HG13	2.00	0.43
2:C:69:LEU:HD12	6:C:302:GOL:H11	2.00	0.43
2:C:69:LEU:HD12	6:C:302:GOL:C1	2.47	0.43
1:L:144:THR:CG2	1:L:146:ILE:H	2.26	0.42
1:L:71:CYS:HG	1:L:79:CYS:CB	2.33	0.42
1:L:228:THR:O	1:L:229:GLY:C	2.57	0.41
3:H:169:TYR:CE1	3:H:193:GLU:HB2	2.55	0.41
2:C:69:LEU:HB2	6:C:302:GOL:C1	2.49	0.41
3:H:160:GLY:CA	7:H:328:HOH:O	2.61	0.41
2:C:180:LEU:HB2	2:C:185:ALA:HB2	2.02	0.41
2:C:80:MET:HE3	7:C:404:HOH:O	2.19	0.41
1:L:133:ARG:NH2	1:L:229:GLY:HA2	2.37	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	L	193/206 (94%)	186 (96%)	7 (4%)	0	100 100
2	C	153/155 (99%)	151 (99%)	2 (1%)	0	100 100
3	H	188/190 (99%)	171 (91%)	16 (8%)	1 (0%)	29 22
All	All	534/551 (97%)	508 (95%)	25 (5%)	1 (0%)	47 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	175	GLY

5.3.2 Protein sidechains (i)

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	L	180/184 (98%)	175 (97%)	5 (3%)	43	44
2	C	141/141 (100%)	137 (97%)	4 (3%)	43	44
3	H	166/166 (100%)	160 (96%)	6 (4%)	35	33
All	All	487/491 (99%)	472 (97%)	15 (3%)	40	39

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	48	THR
1	L	99	VAL
1	L	109	MET
1	L	144	THR
1	L	147	ARG
2	C	88	SER
2	C	125	HIS
2	C	132	ARG
2	C	181	ASP
3	H	63	THR
3	H	119	SER
3	H	121	THR
3	H	153	VAL
3	H	166	LEU
3	H	207	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	126	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	$\#\|Z\| > 2$
4	NAG	A	1	1,4	14,14,15	0.71	0	17,19,21	2.43	6 (35%)
4	NAG	A	2	4	14,14,15	0.59	0	17,19,21	2.53	3 (17%)

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	A	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2	NAG	C1-O5-C5	9.22	124.69	112.19
4	A	1	NAG	O5-C1-C2	-4.83	103.67	111.29
4	A	1	NAG	C1-O5-C5	4.30	118.02	112.19
4	A	1	NAG	C8-C7-N2	3.88	122.68	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1	NAG	O4-C4-C3	-3.58	102.08	110.35
4	A	1	NAG	O4-C4-C5	3.52	118.05	109.30
4	A	1	NAG	O7-C7-N2	-2.76	116.87	121.95
4	A	2	NAG	O5-C1-C2	2.43	115.12	111.29
4	A	2	NAG	C3-C4-C5	2.14	114.05	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

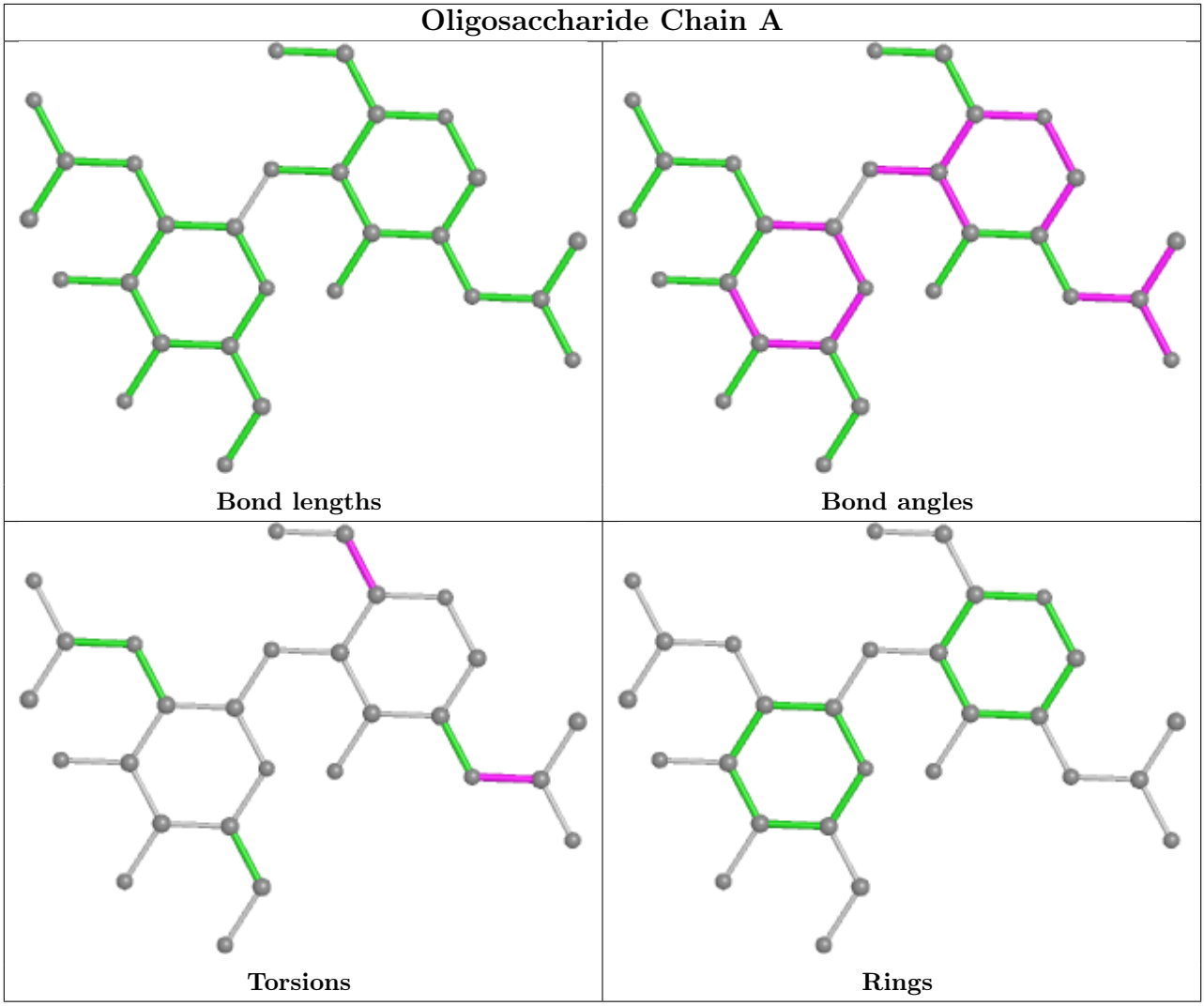
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	1	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)

3 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	$\#\|Z\| > 2$
6	GOL	C	302	-	5,5,5	0.76	0	5,5,5	1.67	1 (20%)
5	NAG	L	303	1	14,14,15	1.12	1 (7%)	17,19,21	2.71	8 (47%)
6	GOL	C	301	-	5,5,5	0.46	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	302	-	-	2/4/4/4	-
5	NAG	L	303	1	-	4/6/23/26	0/1/1/1
6	GOL	C	301	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	303	NAG	O5-C5	2.82	1.49	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	303	NAG	C1-O5-C5	5.49	119.63	112.19
5	L	303	NAG	O5-C5-C6	5.30	115.51	107.20
5	L	303	NAG	C8-C7-N2	4.29	123.36	116.10
5	L	303	NAG	O5-C1-C2	-3.39	105.94	111.29
5	L	303	NAG	C6-C5-C4	-3.11	105.72	113.00
6	C	302	GOL	O3-C3-C2	-3.00	95.82	110.20
5	L	303	NAG	C4-C3-C2	-2.79	106.93	111.02
5	L	303	NAG	C1-C2-N2	2.42	114.61	110.49
5	L	303	NAG	O7-C7-C8	-2.24	117.89	122.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	GOL	O1-C1-C2-C3
5	L	303	NAG	O5-C5-C6-O6
5	L	303	NAG	C4-C5-C6-O6
5	L	303	NAG	C8-C7-N2-C2
5	L	303	NAG	O7-C7-N2-C2
6	C	302	GOL	O1-C1-C2-O2
6	C	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	302	GOL	6	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, 95^{th} 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	L	199/206 (96%)	0.47	23 (11%) 4 6	46, 73, 128, 158	0
2	C	155/155 (100%)	0.16	1 (0%) 89 91	39, 59, 91, 108	0
3	H	190/190 (100%)	0.72	32 (16%) 1 2	41, 79, 149, 173	0
All	All	544/551 (98%)	0.47	56 (10%) 6 9	39, 71, 130, 173	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	176	ALA	9.8
3	H	173	GLU	6.5
3	H	199	ALA	6.4
1	L	152	HIS	6.3
3	H	203	VAL	6.2
3	H	175	GLY	6.1
3	H	174	PRO	5.4
1	L	147	ARG	5.4
1	L	150	ASP	5.2
3	H	170	TRP	5.0
3	H	201	TYR	4.9
3	H	224	VAL	4.5
1	L	101	ALA	4.3
1	L	24	LEU	4.3
1	L	52	VAL	4.2
1	L	148	ALA	4.1
3	H	200	ALA	4.0
1	L	50	ASP	3.9
1	L	151	GLY	3.8
1	L	99	VAL	3.8
3	H	36	PRO	3.8
3	H	172	ARG	3.7
3	H	150	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	H	177	GLU	3.6
1	L	149	GLY	3.6
2	C	206	LEU	3.6
3	H	202	CYS	3.6
3	H	169	TYR	3.5
1	L	48	THR	3.4
1	L	49	PRO	3.3
3	H	119	SER	3.3
3	H	171	ARG	3.3
3	H	91	LEU	3.2
3	H	195	MET	3.1
3	H	60	PRO	3.0
1	L	105	SER	3.0
1	L	98	ALA	2.9
3	H	168	ALA	2.9
3	H	198	GLY	2.8
3	H	178	GLU	2.8
3	H	197	PRO	2.7
3	H	148	ASP	2.6
3	H	59	ALA	2.6
3	H	223	CYS	2.6
1	L	225	ARG	2.5
1	L	73	ARG	2.5
3	H	65	TYR	2.4
1	L	76	ARG	2.3
1	L	69	LYS	2.2
3	H	149	GLY	2.2
1	L	153	ARG	2.2
1	L	75	THR	2.2
3	H	57	VAL	2.2
1	L	154	LEU	2.1
3	H	117	LEU	2.1
1	L	74	ILE	2.1

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

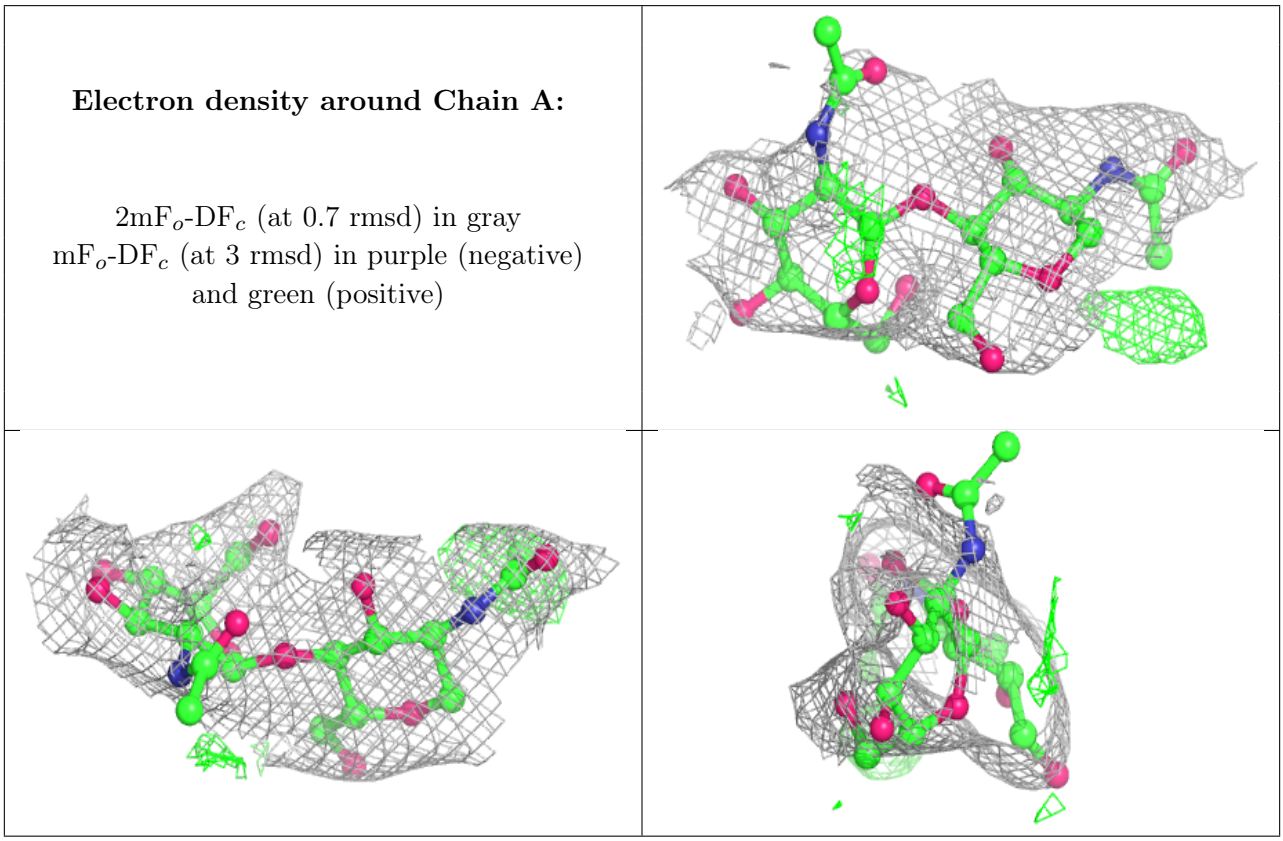
There are no non-standard protein/DNA/RNA residues in this entry.

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	2	14/15	0.81	0.32	118,134,143,147	0
4	NAG	A	1	14/15	0.97	0.11	96,106,117,120	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^{th} 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
5	NAG	L	303	14/15	0.79	0.17	99,111,122,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	301	6/6	0.91	0.19	78,87,91,91	0
6	GOL	C	302	6/6	0.93	0.32	36,39,41,49	6

6.5 Other polymers (i)

There are no such residues in this entry.