W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2023 – 12:51 PM EST

PDB ID	:	4GRW
Title	:	Structure of a complex of human IL-23 with 3 Nanobodies (Llama vHHs)
Authors	:	Desmyter, A.; Spinelli, S.; Button, C.; Saunders, M.; de Haard, H.; Rommelaere, H.; Union, A.; Cambillau, C.
Deposited on	:	2012-08-27
Resolution	:	2.55 Å(reported)

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

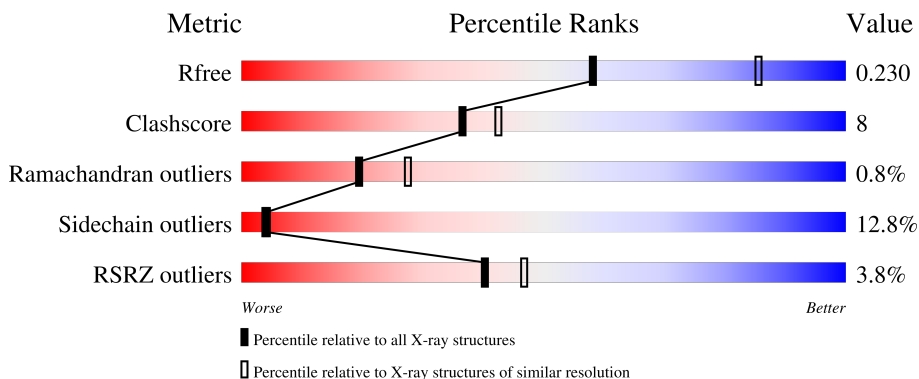|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		8
Ramachandran outliers		0.8%
Sidechain outliers		12.8%
RSRZ outliers		3.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	A	189	3% 52% 12% 5% 31%
1	C	189	.% 63% · · 32%
2	B	328	2% 71% 15% · 11%
2	D	328	2% 71% 14% · 11%
3	E	125	81% 18% ·

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Mol	Chain	Length	Quality of chain
3	G	125	% 83% 15% ·
4	F	126	6% 71% 25% · ·
4	J	126	20% 60% 29% 6% · ·
5	H	123	2% 76% 19% 6%
5	I	123	2% 77% 19% ·
6	K	5	80% 20%
6	L	5	40% 60%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 13131 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-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1010	647	181	177	5			
1	C	129	Total	C	N	O	S	0	0	0
			1002	643	179	175	5			

- Molecule 2 is a protein called Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	0	0	0
			2331	1478	382	459	12			
2	D	292	Total	C	N	O	S	0	0	0
			2319	1467	379	461	12			

- Molecule 3 is a protein called Nanobody 124C4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	125	Total	C	N	O	S	0	0	0
			938	586	161	187	4			
3	G	125	Total	C	N	O	S	0	0	0
			937	586	161	186	4			

- Molecule 4 is a protein called Nanobody 37D5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	125	Total	C	N	O	S	0	0	0
			954	596	161	192	5			
4	J	122	Total	C	N	O	S	0	0	0
			932	583	158	186	5			

- Molecule 5 is a protein called Nanobody 22E11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	123	Total 938	C 585	N 168	O 182	S 3	0	0	0
5	I	123	Total 938	C 585	N 168	O 182	S 3	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
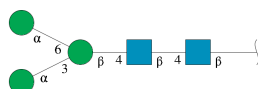
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	5	Total 61	C 34	N 2	O 25	0	0	0
6	L	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total 24	O 24	0	0
7	B	143	Total 143	O 143	0	0
7	C	48	Total 48	O 48	0	0
7	D	187	Total 187	O 187	0	0
7	E	67	Total 67	O 67	0	0
7	F	38	Total 38	O 38	0	0
7	G	57	Total 57	O 57	0	0
7	H	50	Total 50	O 50	0	0
7	I	73	Total 73	O 73	0	0
7	J	23	Total 23	O 23	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.
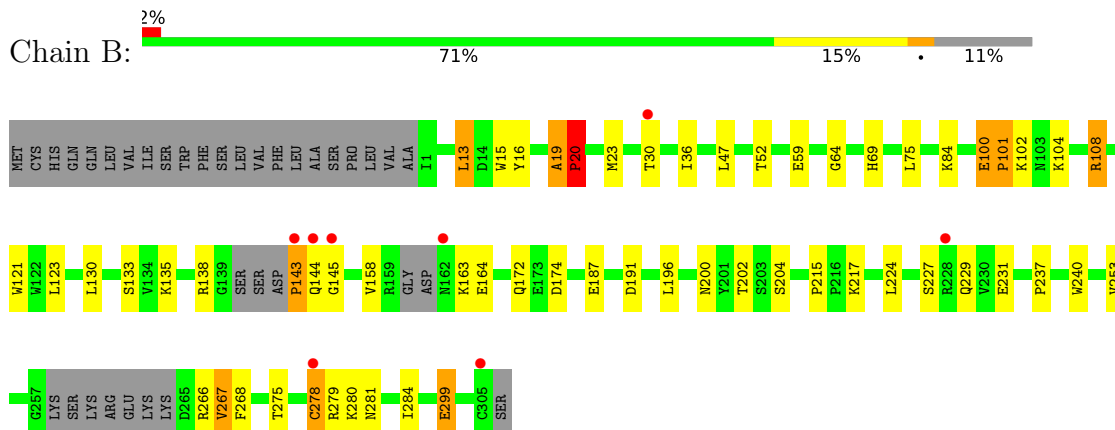
- Molecule 1: Interleukin-23 subunit alpha
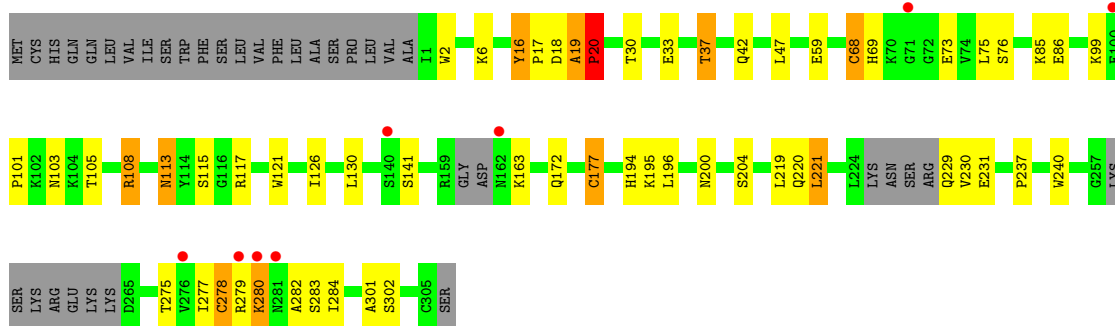

Chain A:

- Molecule 1: Interleukin-23 subunit alpha
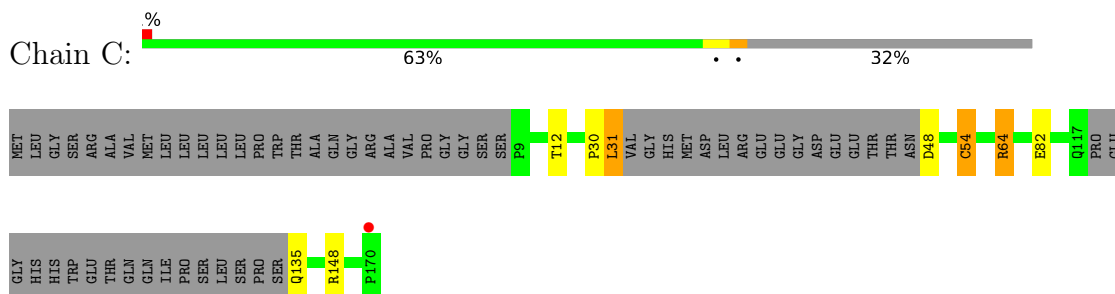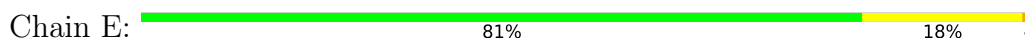

Chain C:

- Molecule 2: Interleukin-12 subunit beta

Chain B:

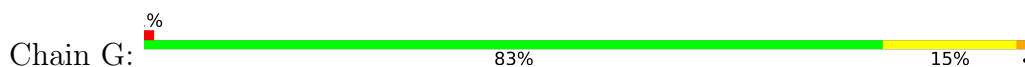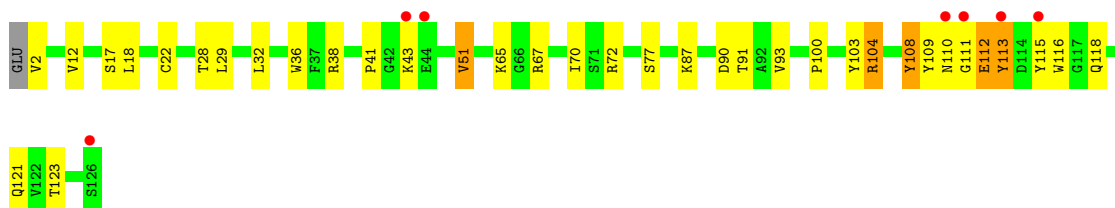- Molecule 2: Interleukin-12 subunit beta

Chain D:

- Molecule 3: Nanobody 124C4

Chain E:

- Molecule 3: Nanobody 124C4

Chain G:

- Molecule 4: Nanobody 37D5

Chain F:

- Molecule 4: Nanobody 37D5

Chain J:

- Molecule 5: Nanobody 22E11

Chain H:

• Molecule 5: Nanobody 22E11

Chain I:

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

Chain K:

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

Chain L:
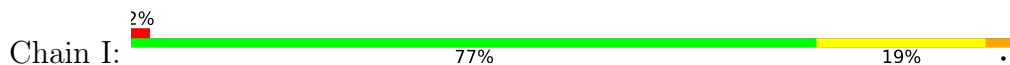
4 Data and refinement statistics (i)

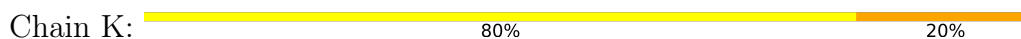| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.27Å 135.14Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.83 – 2.55 43.83 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.83-2.55) 99.8 (43.83-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.183 , 0.218 0.192 , 0.230	Depositor DCC
R_{free} test set	1940 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13131	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.55	0/1034	0.73	1/1405 (0.1%)
1	C	0.50	0/1026	0.65	0/1393
2	B	0.50	0/2387	0.75	1/3241 (0.0%)
2	D	0.52	2/2375 (0.1%)	0.72	0/3228
3	E	0.54	0/958	0.73	0/1300
3	G	0.51	0/957	0.77	0/1299
4	F	0.54	0/975	0.69	0/1323
4	J	0.55	0/952	0.77	1/1290 (0.1%)
5	H	0.56	0/960	0.71	0/1302
5	I	0.49	0/960	0.68	0/1302
All	All	0.53	2/12584 (0.0%)	0.72	3/17083 (0.0%)

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	3
2	B	0	1
4	F	0	2
4	J	0	7
5	H	0	2
5	I	0	1
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	20	PRO	N-CD	5.53	1.55	1.47
2	D	16	TYR	CE1-CZ	-5.03	1.32	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	110	ASN	C-N-CA	6.78	136.53	122.30
1	A	29	HIS	C-N-CD	5.85	140.69	128.40
2	B	20	PRO	CA-N-CD	-5.54	103.75	111.50

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ALA	Peptide
1	A	30	PRO	Peptide
1	A	47	ASN	Peptide
2	B	143	PRO	Peptide
4	F	112	GLU	Peptide

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	1010	0	1006	31	0
1	C	1002	0	1001	5	0
2	B	2331	0	2244	31	0
2	D	2319	0	2215	37	0
3	E	938	0	890	8	0
3	G	937	0	887	9	0
4	F	954	0	888	30	0
4	J	932	0	869	25	0
5	H	938	0	893	11	0
5	I	938	0	893	16	0
6	K	61	0	52	3	0
6	L	61	0	52	7	0
7	A	24	0	0	0	0
7	B	143	0	0	1	0
7	C	48	0	0	1	0
7	D	187	0	0	2	0
7	E	67	0	0	0	0
7	F	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	57	0	0	0	0
7	H	50	0	0	0	0
7	I	73	0	0	1	0
7	J	23	0	0	0	0
All	All	13131	0	11890	189	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.

The worst 5 of 189 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:D:200:ASN:HD21	6:L:1:NAG:C1	1.31	1.44
2:B:200:ASN:HD21	6:K:1:NAG:C1	1.36	1.30
4:J:22:CYS:SG	4:J:96:CYS:SG	1.30	1.29
1:A:137:TRP:HB3	1:A:138:GLN:HB3	1.18	1.18
1:A:137:TRP:HB3	1:A:138:GLN:CB	1.79	1.11

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	124/189 (66%)	118 (95%)	2 (2%)	4 (3%)	4	3
1	C	123/189 (65%)	120 (98%)	3 (2%)	0	100	100
2	B	285/328 (87%)	269 (94%)	14 (5%)	2 (1%)	22	30
2	D	284/328 (87%)	268 (94%)	13 (5%)	3 (1%)	14	19
3	E	123/125 (98%)	123 (100%)	0	0	100	100
3	G	123/125 (98%)	122 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	123/126 (98%)	118 (96%)	5 (4%)	0	100	100
4	J	118/126 (94%)	109 (92%)	7 (6%)	2 (2%)	9	11
5	H	121/123 (98%)	118 (98%)	2 (2%)	1 (1%)	19	27
5	I	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
All	All	1545/1782 (87%)	1485 (96%)	48 (3%)	12 (1%)	19	27

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	136	PRO
2	B	19	ALA
2	D	19	ALA
4	J	116	TRP

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	109/159 (69%)	99 (91%)	10 (9%)	9	11
1	C	108/159 (68%)	101 (94%)	7 (6%)	17	23
2	B	263/297 (89%)	235 (89%)	28 (11%)	6	7
2	D	262/297 (88%)	233 (89%)	29 (11%)	6	6
3	E	96/97 (99%)	82 (85%)	14 (15%)	3	2
3	G	95/97 (98%)	85 (90%)	10 (10%)	7	7
4	F	100/103 (97%)	86 (86%)	14 (14%)	3	3
4	J	97/103 (94%)	72 (74%)	25 (26%)	0	0
5	H	98/99 (99%)	78 (80%)	20 (20%)	1	1
5	I	98/99 (99%)	85 (87%)	13 (13%)	4	3
All	All	1326/1510 (88%)	1156 (87%)	170 (13%)	4	4

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	H	13	GLN
5	I	104	THR
5	H	38	ARG
5	H	120	THR
4	J	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	200	ASN
3	E	82	GLN
5	I	39	GLN
3	E	77	ASN
4	F	82	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	K	1	6,2	14,14,15	0.38	0	17,19,21	2.40	5 (29%)
6	NAG	K	2	6	14,14,15	0.44	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	BMA	K	3	6	11,11,12	0.47	0	15,15,17	1.19	1 (6%)
6	MAN	K	4	6	11,11,12	0.51	0	15,15,17	1.34	2 (13%)
6	MAN	K	5	6	11,11,12	0.49	0	15,15,17	1.29	3 (20%)
6	NAG	L	1	6,2	14,14,15	0.38	0	17,19,21	2.44	4 (23%)
6	NAG	L	2	6	14,14,15	0.45	0	17,19,21	1.04	2 (11%)
6	BMA	L	3	6	11,11,12	0.41	0	15,15,17	1.44	2 (13%)
6	MAN	L	4	6	11,11,12	0.48	0	15,15,17	1.25	3 (20%)
6	MAN	L	5	6	11,11,12	0.43	0	15,15,17	1.44	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
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	2/2/19/22	0/1/1/1
6	MAN	K	5	6	-	2/2/19/22	0/1/1/1
6	NAG	L	1	6,2	-	5/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1	NAG	C2-N2-C7	6.52	132.19	122.90
6	K	1	NAG	C1-C2-N2	-5.93	100.35	110.49
6	L	1	NAG	C4-C3-C2	-5.90	102.38	111.02
6	K	1	NAG	O5-C1-C2	4.77	118.82	111.29
6	L	5	MAN	C1-O5-C5	4.57	118.38	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	5	MAN	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	K	5	MAN	O5-C5-C6-O6
6	K	3	BMA	O5-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	3	BMA	1	0
6	K	1	NAG	3	0
6	L	5	MAN	1	0
6	L	1	NAG	6	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 K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings
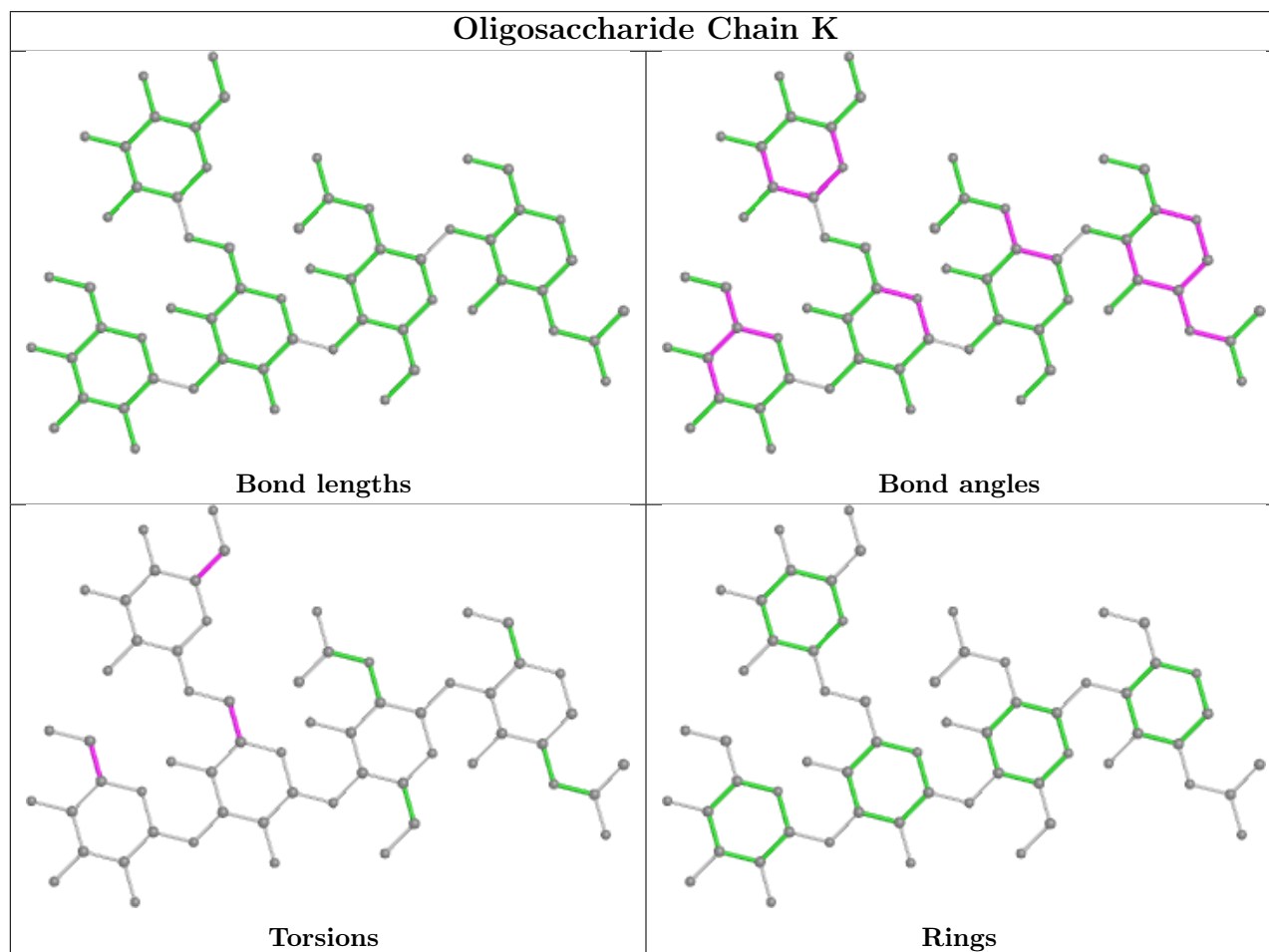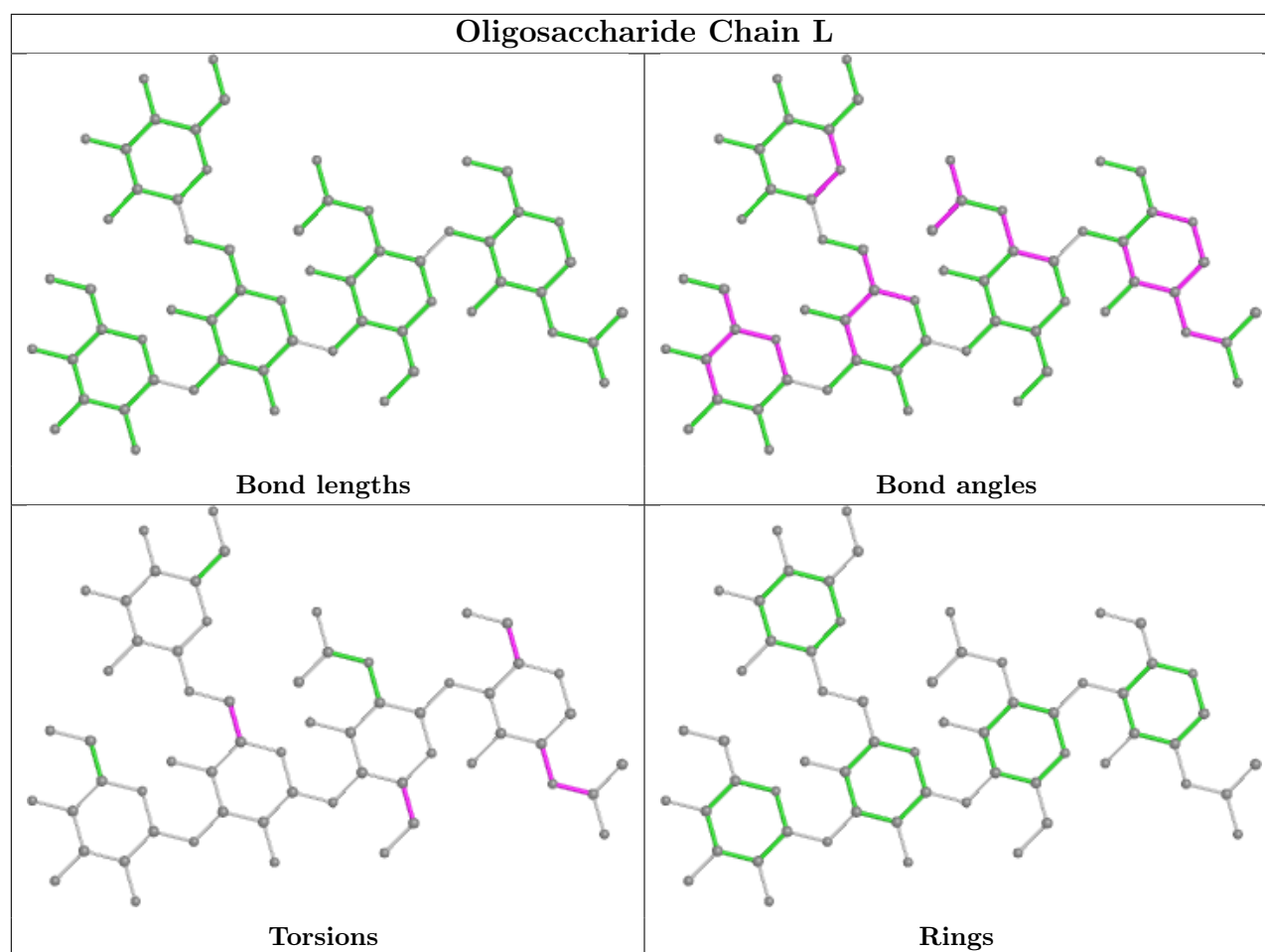
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	A	130/189 (68%)	0.25	6 (4%)	32	39	33, 54, 87, 109	0
1	C	129/189 (68%)	0.05	1 (0%)	86	89	29, 42, 68, 102	0
2	B	293/328 (89%)	0.07	8 (2%)	54	61	28, 45, 83, 126	0
2	D	292/328 (89%)	0.01	8 (2%)	54	61	24, 40, 84, 130	0
3	E	125/125 (100%)	-0.30	0	100	100	26, 37, 55, 94	0
3	G	125/125 (100%)	-0.23	1 (0%)	86	89	33, 44, 63, 109	0
4	F	125/126 (99%)	0.16	7 (5%)	24	29	28, 51, 85, 113	0
4	J	122/126 (96%)	1.14	25 (20%)	1	1	40, 73, 102, 118	0
5	H	123/123 (100%)	0.07	2 (1%)	72	78	28, 48, 78, 100	0
5	I	123/123 (100%)	0.03	2 (1%)	72	78	25, 41, 68, 104	0
All	All	1587/1782 (89%)	0.10	60 (3%)	40	47	24, 45, 86, 130	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	126	SER	5.4
4	J	41	PRO	5.4
2	D	100	GLU	4.9
2	D	280	LYS	4.9
2	B	144	GLN	4.6

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	MAN	K	5	11/12	0.50	0.33	84,130,146,150	0
6	MAN	K	4	11/12	0.57	0.26	62,92,147,148	0
6	MAN	L	5	11/12	0.79	0.33	81,105,128,138	0
6	BMA	K	3	11/12	0.84	0.18	51,106,130,136	0
6	MAN	L	4	11/12	0.88	0.15	43,98,120,127	0
6	BMA	L	3	11/12	0.92	0.17	54,95,123,128	0
6	NAG	L	1	14/15	0.93	0.15	16,40,89,96	0
6	NAG	K	1	14/15	0.96	0.12	20,44,57,82	0
6	NAG	L	2	14/15	0.97	0.13	25,41,58,76	0
6	NAG	K	2	14/15	0.97	0.14	24,39,72,93	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.

Electron density around Chain K:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain L:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
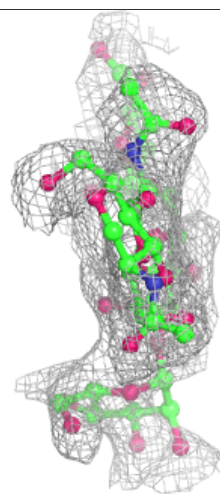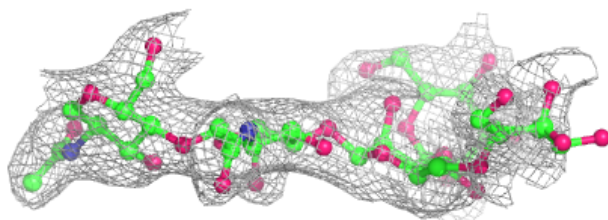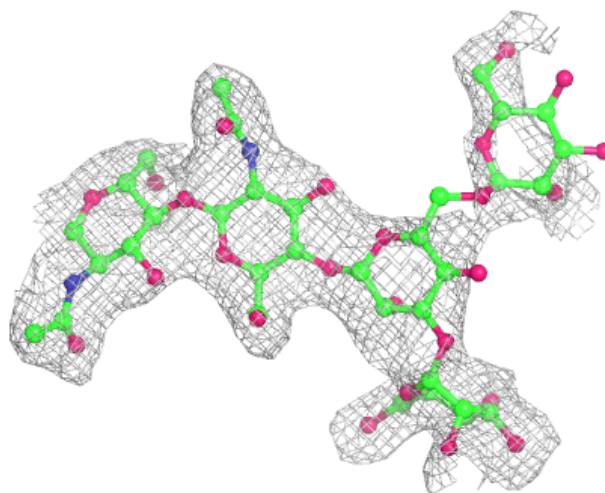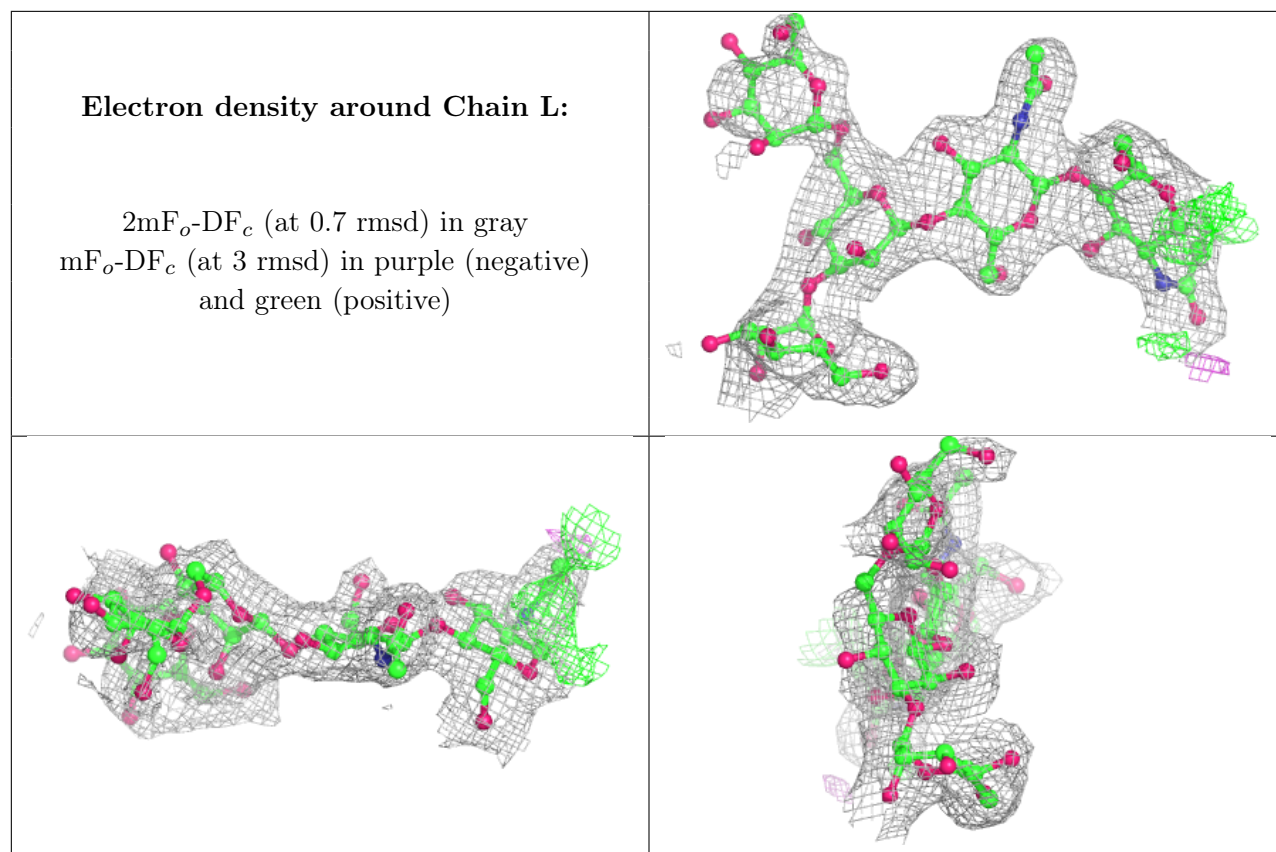
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.