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)

Sep 25, 2023 – 11:38 PM EDT

PDB ID	:	6BGA
Title	:	2B4 I-Ek TCR-MHC complex with affinity-enhancing Velcro peptide
Authors	:	Gee, M.H.; Sibener, L.V.; Birnbaum, M.E.; Jude, K.M.; Garcia, K.C.
Deposited on	:	2017-10-27
Resolution	:	2.31 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) 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 2.31 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.
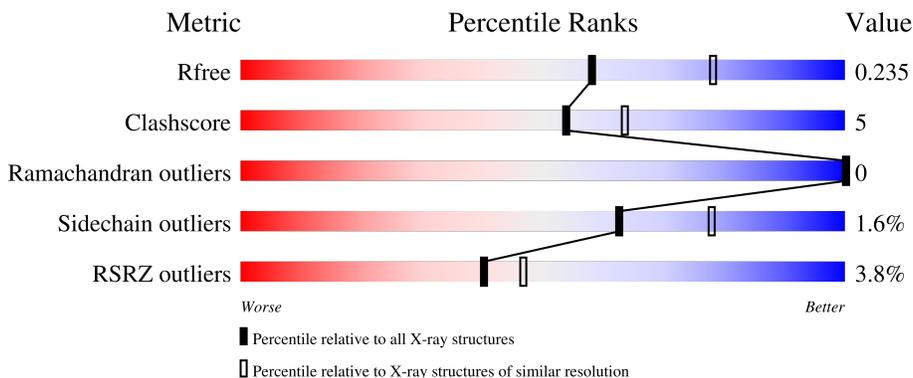
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	204	% 78% 11% 11%
2	B	233	% 75% 13% • 11%
3	C	220	7% 77% 13% • 10%
4	D	255	5% 85% 11% •
5	E	15	40% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	2	50% 50%
6	G	2	100%
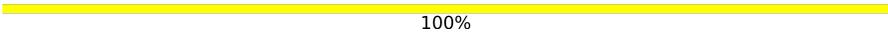
2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 7233 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 H-2 class II histocompatibility antigen, E-K alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1491	961	245	281	4			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P04224
A	-1	ASP	-	expression tag	UNP P04224
A	0	PRO	-	expression tag	UNP P04224
A	192	SER	-	expression tag	UNP P04224
A	193	ARG	-	expression tag	UNP P04224
A	194	GLY	-	expression tag	UNP P04224
A	195	GLY	-	expression tag	UNP P04224
A	196	LEU	-	expression tag	UNP P04224
A	197	GLU	-	expression tag	UNP P04224
A	198	VAL	-	expression tag	UNP P04224
A	199	LEU	-	expression tag	UNP P04224
A	200	PHE	-	expression tag	UNP P04224
A	201	GLN	-	expression tag	UNP P04224

- Molecule 2 is a protein called 2B4 peptide,MHC I-Ek B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1660	1051	285	318	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	SER	-	expression tag	UNP Q31163
B	200	ARG	-	expression tag	UNP Q31163
B	201	GLY	-	expression tag	UNP Q31163

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	GLY	-	expression tag	UNP Q31163
B	203	LEU	-	expression tag	UNP Q31163
B	204	GLU	-	expression tag	UNP Q31163
B	205	VAL	-	expression tag	UNP Q31163
B	206	LEU	-	expression tag	UNP Q31163
B	207	PHE	-	expression tag	UNP Q31163
B	208	GLN	-	expression tag	UNP Q31163

- Molecule 3 is a protein called T cell receptor 2B4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	199	Total 1534	C 950	N 263	O 313	S 8	0	0	0

- Molecule 4 is a protein called T cell receptor 2B4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total 1975	C 1247	N 342	O 377	S 9	0	1	0

- Molecule 5 is a protein called Velcro peptide.

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	6	Total 48	C 33	N 6	O 9	0	0	0

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

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	2	Total 24	C 14	N 1	O 9	0	0	0
6	G	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
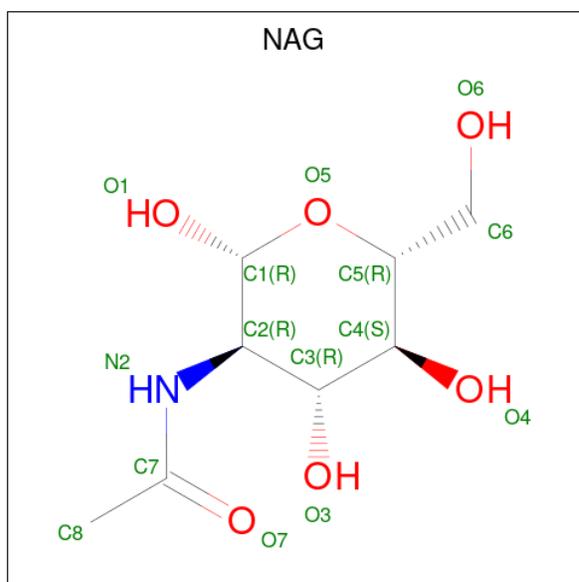
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 14	C 8	N 1	O 5	0	0
7	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
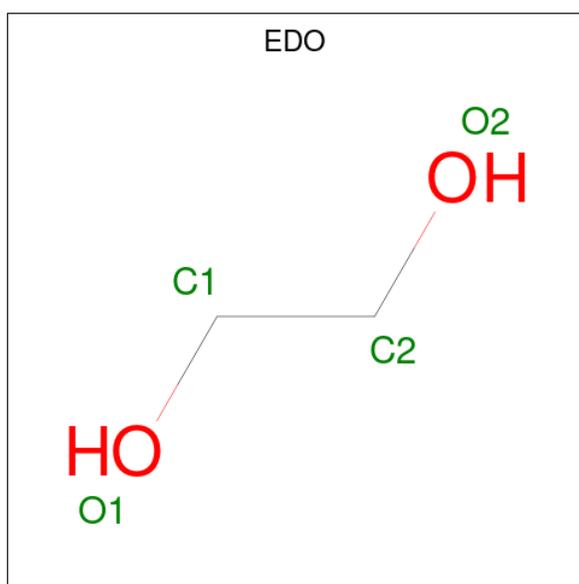
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 4	C 2	O 2	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
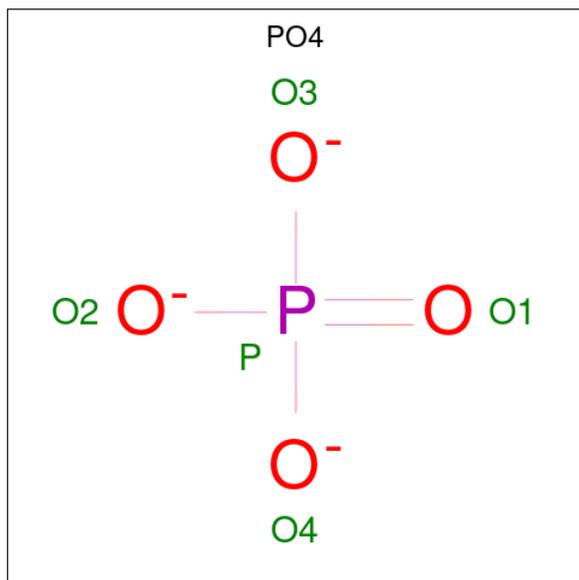
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total 5	O 4	P 1	0	0

- Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	124	Total 124	O 124	0	0
10	B	129	Total 129	O 129	0	0
10	C	67	Total 67	O 67	0	0
10	D	104	Total 104	O 104	0	0
10	E	8	Total 8	O 8	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: H-2 class II histocompatibility antigen, E-K alpha chain
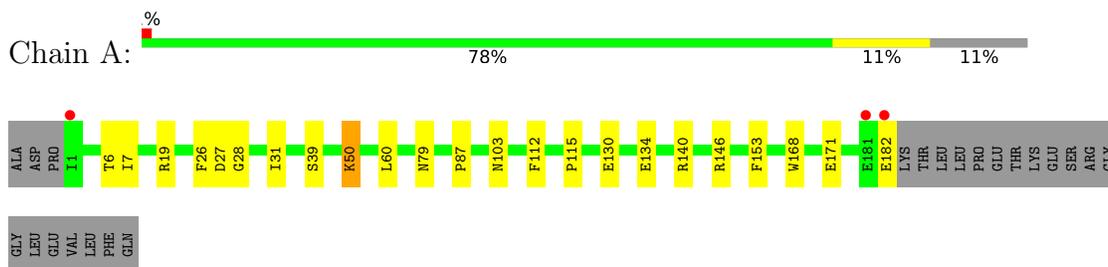
Chain A:

• Molecule 2: 2B4 peptide,MHC I-Ek B chain
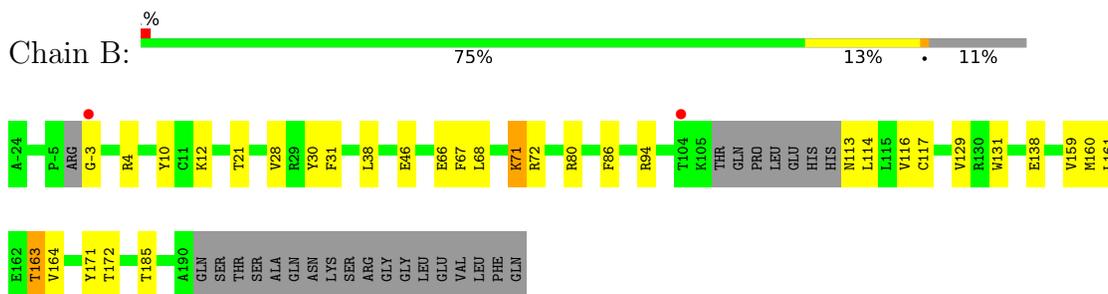
Chain B:

• Molecule 3: T cell receptor 2B4 alpha chain
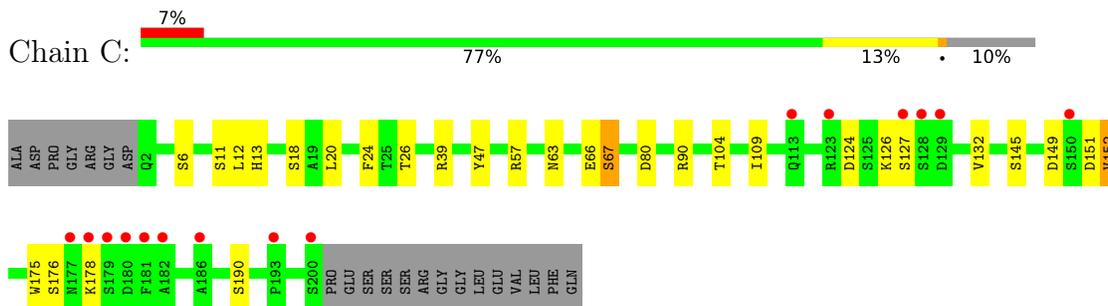
Chain C:

• Molecule 4: T cell receptor 2B4 beta chain

Chain D:

N220 D221 E222 W223 T224 Q225 D226 R227 A228 A237 D244 SER ARG GLY GLY LEU GLU VAL LEU PHE GLN
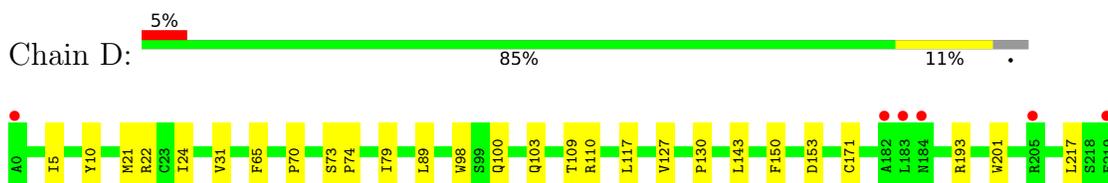
- Molecule 5: Velcro peptide
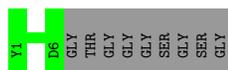
Chain E:

40%   60%

Y1 D6 GLY THR GLY GLY SER GLY SER GLY

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

50%   50%

NAG1 FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

100%

NAG1 FUC2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	79.11Å 58.85Å 224.62Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	47.21 – 2.31 47.21 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.21-2.31) 97.3 (47.21-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.192 , 0.237 0.192 , 0.235	Depositor DCC
R_{free} test set	2163 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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, FUC, PO4, EDO

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	0.25	0/1534	0.45	0/2086
2	B	0.25	0/1702	0.43	0/2312
3	C	0.26	0/1563	0.45	0/2117
4	D	0.26	0/2028	0.43	0/2758
5	E	0.25	0/49	0.43	0/68
All	All	0.25	0/6876	0.44	0/9341

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	A	1491	0	1413	16	0
2	B	1660	0	1569	28	0
3	C	1534	0	1448	17	0
4	D	1975	0	1886	18	0
5	E	48	0	49	0	0
6	F	24	0	22	2	0
6	G	24	0	22	0	0
7	A	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	8	0	12	1	0
8	B	4	0	6	0	0
9	B	5	0	0	1	0
10	A	124	0	0	2	0
10	B	129	0	0	3	0
10	C	67	0	0	0	0
10	D	104	0	0	1	0
10	E	8	0	0	0	0
All	All	7233	0	6453	70	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.

The worst 5 of 70 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:C:151:ASP:HB2	3:C:178:LYS:HD2	1.71	0.73
2:B:21:THR:O	2:B:80:ARG:NH1	2.28	0.67
1:A:27:ASP:HB3	8:A:304:EDO:H22	1.78	0.65
2:B:114:LEU:HD22	2:B:160:MET:HB3	1.81	0.62
2:B:10:TYR:HB3	2:B:31:PHE:HB2	1.82	0.61

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/204 (88%)	175 (97%)	5 (3%)	0	100	100
2	B	201/233 (86%)	194 (96%)	7 (4%)	0	100	100
3	C	197/220 (90%)	196 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	244/255 (96%)	234 (96%)	10 (4%)	0	100	100
5	E	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
All	All	826/927 (89%)	802 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	163/184 (89%)	159 (98%)	4 (2%)	47	65
2	B	183/208 (88%)	180 (98%)	3 (2%)	62	78
3	C	173/191 (91%)	170 (98%)	3 (2%)	60	76
4	D	218/225 (97%)	216 (99%)	2 (1%)	78	89
5	E	6/9 (67%)	6 (100%)	0	100	100
All	All	743/817 (91%)	731 (98%)	12 (2%)	62	78

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	6	SER
3	C	67	SER
4	D	193	ARG
3	C	152	VAL
1	A	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 ⓘ

4 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	F	1	2,6	14,14,15	0.37	0	17,19,21	0.37	0
6	FUC	F	2	6	10,10,11	1.35	2 (20%)	14,14,16	1.19	1 (7%)
6	NAG	G	1	6,3	14,14,15	0.83	1 (7%)	17,19,21	0.55	0
6	FUC	G	2	6	10,10,11	0.85	0	14,14,16	1.01	1 (7%)

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	F	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	F	2	6	-	-	0/1/1/1
6	NAG	G	1	6,3	-	2/6/23/26	0/1/1/1
6	FUC	G	2	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1	NAG	O5-C1	-2.40	1.39	1.43
6	F	2	FUC	C2-C3	2.40	1.56	1.52
6	F	2	FUC	O5-C1	-2.12	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	2	FUC	C1-C2-C3	2.56	112.81	109.67
6	G	2	FUC	O2-C2-C1	2.30	113.85	109.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	1	NAG	C4-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	2	FUC	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 F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
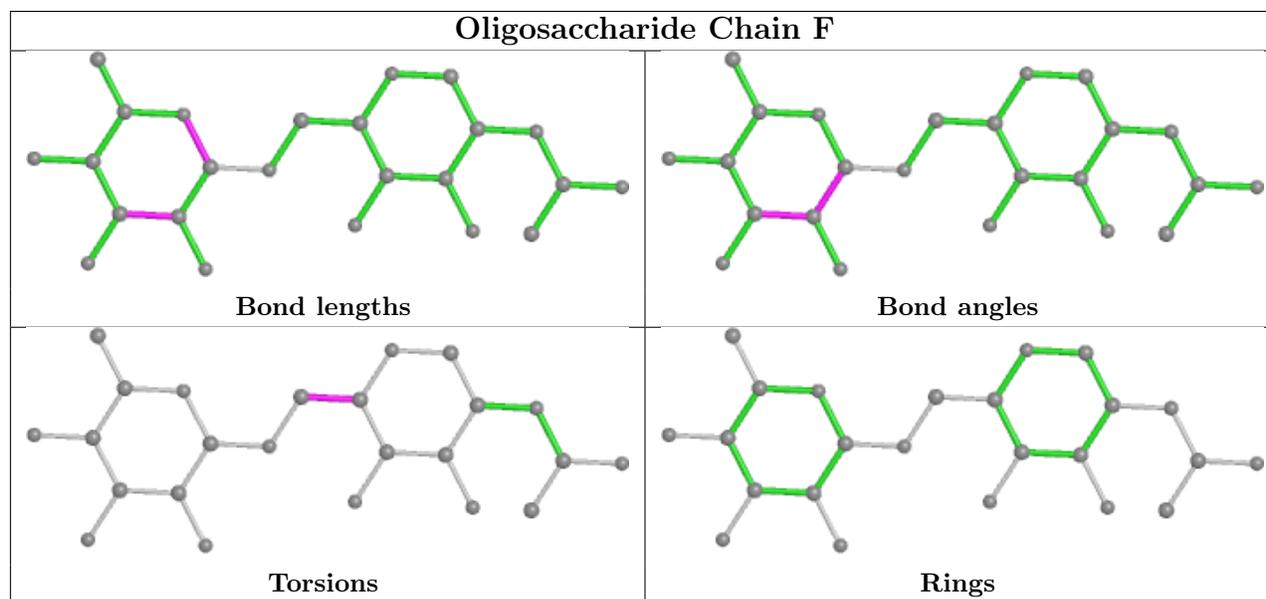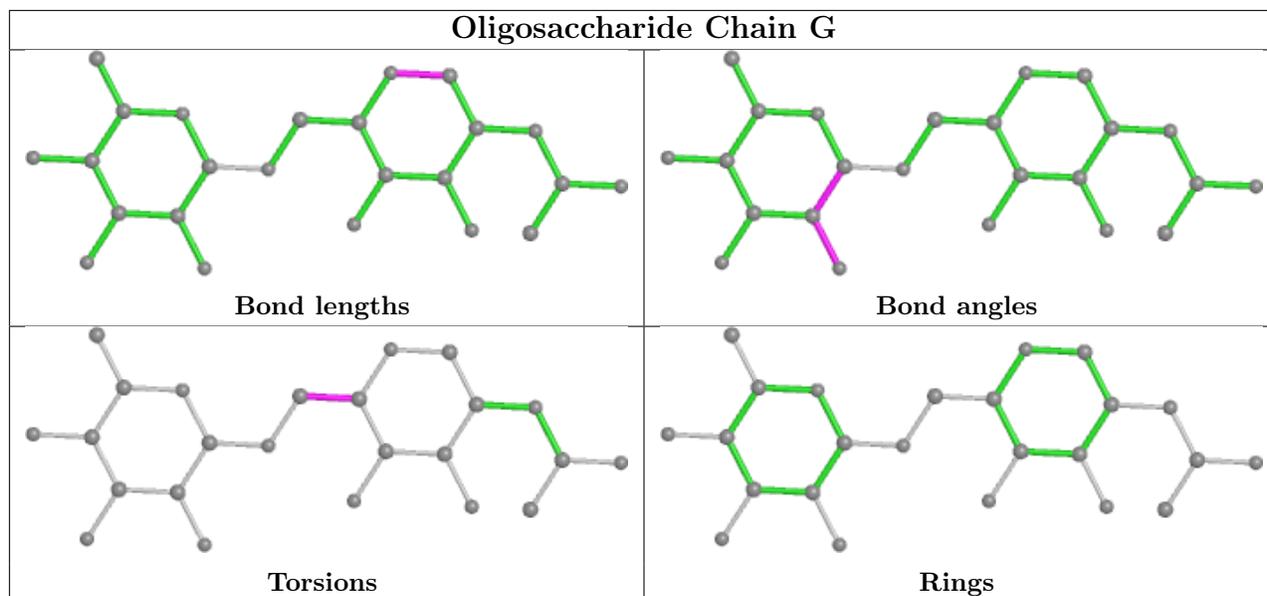
5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
7	NAG	A	301	1	14,14,15	0.23	0	17,19,21	0.35	0
8	EDO	A	304	-	3,3,3	0.44	0	2,2,2	0.37	0
8	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.39	0
9	PO4	B	304	-	4,4,4	0.92	0	6,6,6	0.43	0
7	NAG	A	302	1	14,14,15	0.39	0	17,19,21	0.36	0
8	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	301	1	-	2/6/23/26	0/1/1/1
8	EDO	A	304	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	303	-	-	0/1/1/1	-
7	NAG	A	302	1	-	0/6/23/26	0/1/1/1
8	EDO	A	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	301	NAG	O5-C5-C6-O6
7	A	301	NAG	C4-C5-C6-O6
8	A	303	EDO	O1-C1-C2-O2
8	A	304	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	304	EDO	1	0
9	B	304	PO4	1	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(Å²)	Q<0.9
1	A	182/204 (89%)	0.01	3 (1%)	72	77	21, 32, 62, 90	0
2	B	207/233 (88%)	0.12	2 (0%)	82	86	20, 31, 69, 94	0
3	C	199/220 (90%)	0.29	15 (7%)	14	19	25, 46, 106, 125	0
4	D	245/255 (96%)	0.10	12 (4%)	29	36	21, 43, 88, 135	0
5	E	6/15 (40%)	-0.06	0	100	100	32, 34, 39, 62	0
All	All	839/927 (90%)	0.13	32 (3%)	40	47	20, 39, 88, 135	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	181	PHE	6.7
4	D	224	THR	6.5
4	D	226	ASP	4.8
3	C	179	SER	4.7
3	C	129	ASP	4.3

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 ⓘ

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(Å²)	Q<0.9
6	NAG	G	1	14/15	0.75	0.24	54,69,77,80	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	F	1	14/15	0.78	0.23	64,72,74,74	0
6	FUC	F	2	10/11	0.81	0.29	70,76,79,80	0
6	FUC	G	2	10/11	0.86	0.30	87,91,92,93	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.
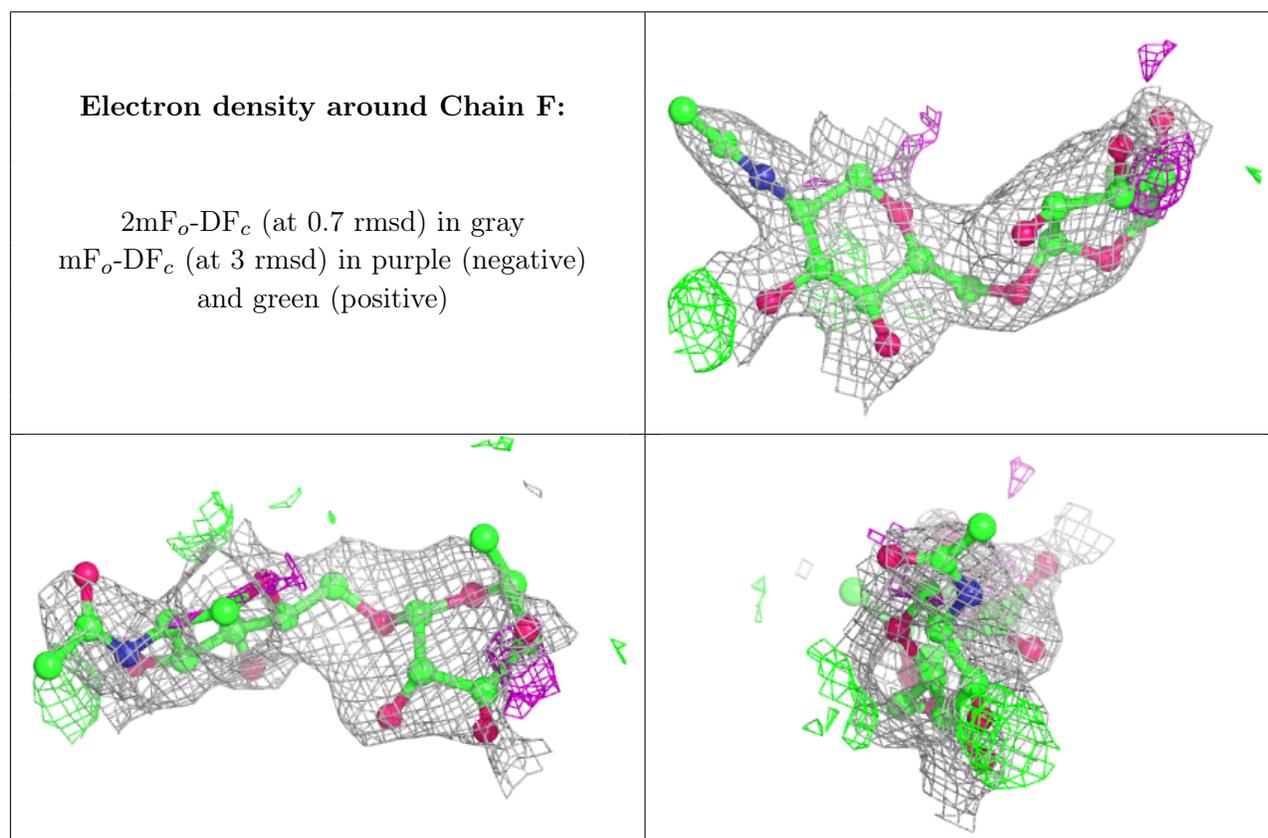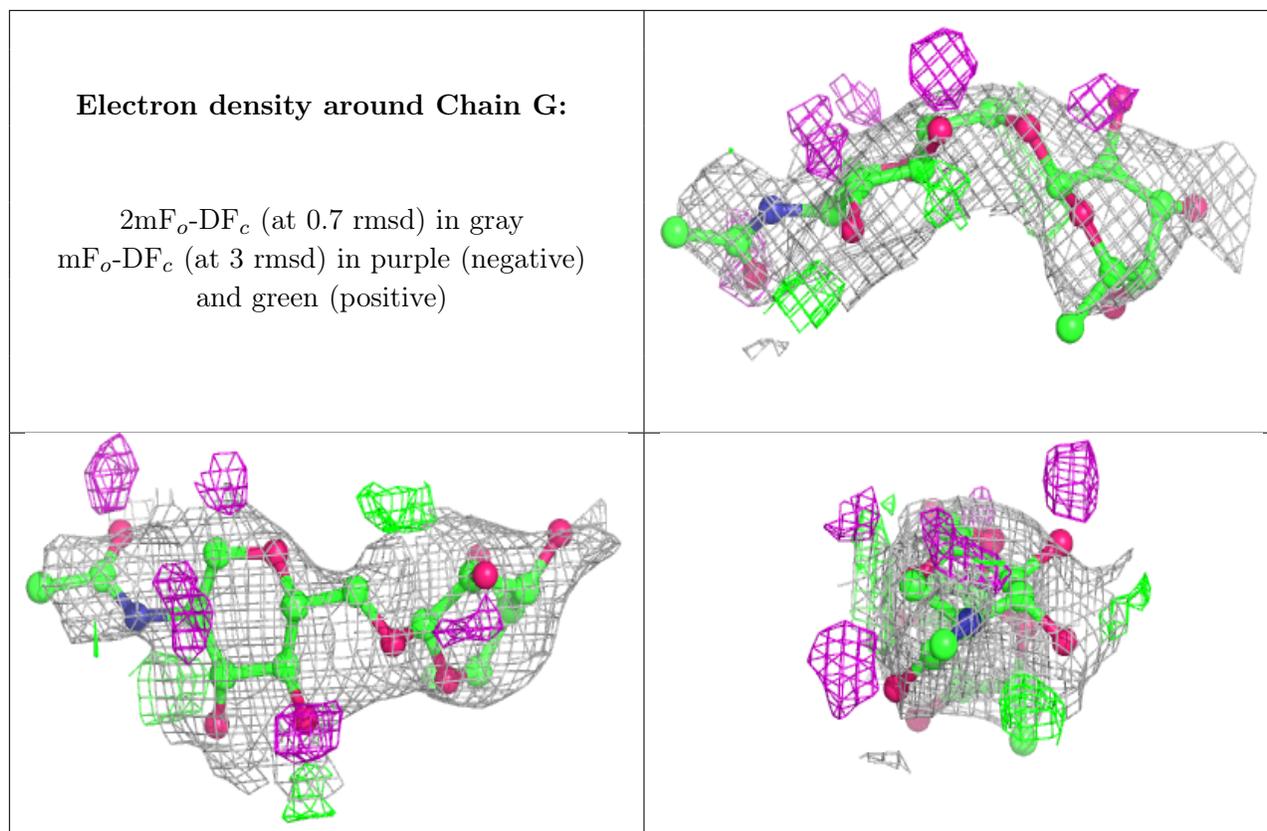
Electron density around Chain F:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain G:

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

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	NAG	A	301	14/15	0.62	0.28	77,86,87,89	0
7	NAG	A	302	14/15	0.77	0.26	63,75,81,84	0
8	EDO	A	304	4/4	0.80	0.29	45,51,53,54	0
9	PO4	B	304	5/5	0.90	0.29	103,106,107,108	0
8	EDO	B	303	4/4	0.94	0.17	42,43,45,46	0
8	EDO	A	303	4/4	0.94	0.13	53,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.