



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:12 PM UTC

PDB ID : 7SEG / pdb_00007seg
Title : Crystal structure of the complex of CD16A bound by an anti-CD16A Fab
Authors : Kiefer, J.R.; Wallweber, H.A.; Polson, A.G.
Deposited on : 2021-09-30
Resolution : 2.16 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

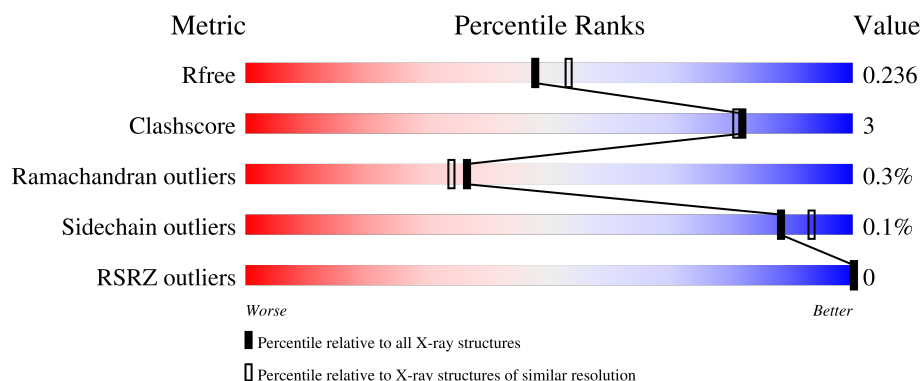
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	236	 86% 11%
1	L	236	 82% 7% 11%
2	A	247	 83% 13%
2	H	247	 80% 7% 13%
3	C	180	 88% 5% 7%

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Mol	Chain	Length	Quality of chain
3	D	180	 85%8%7%
4	E	2	 50%50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9357 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 anti-CD16a Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1594	993	274	322	5			
1	B	211	Total	C	N	O	S	0	0	0
			1598	995	274	324	5			

- Molecule 2 is a protein called anti-CD16A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	1	0
			1620	1030	259	322	9			
2	A	216	Total	C	N	O	S	0	0	0
			1624	1032	263	320	9			

- Molecule 3 is a protein called Low affinity immunoglobulin gamma Fc region receptor III-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	167	Total	C	N	O	S	0	1	0
			1339	855	227	253	4			
3	C	167	Total	C	N	O	S	0	0	0
			1308	831	226	247	4			

There are 14 discrepancies between the modelled and reference sequences:

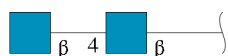
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	MET	conflict	UNP P08637
D	35	GLN	ASN	conflict	UNP P08637
D	71	GLN	ASN	conflict	UNP P08637
D	155	VAL	PHE	variant	UNP P08637
D	166	GLN	ASN	conflict	UNP P08637
D	173	GLY	-	expression tag	UNP P08637
D	174	ASN	-	expression tag	UNP P08637
C	-3	SER	MET	conflict	UNP P08637

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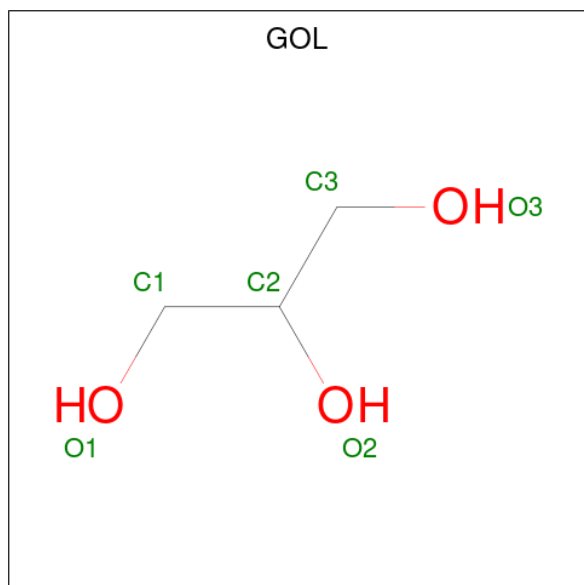
Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLN	ASN	conflict	UNP P08637
C	71	GLN	ASN	conflict	UNP P08637
C	155	VAL	PHE	variant	UNP P08637
C	166	GLN	ASN	conflict	UNP P08637
C	173	GLY	-	expression tag	UNP P08637
C	174	ASN	-	expression tag	UNP P08637

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	23	Total	O	0	0
			23	23		
7	H	50	Total	O	0	0
			50	50		
7	B	31	Total	O	0	0
			31	31		
7	A	48	Total	O	0	0
			48	48		
7	D	25	Total	O	0	0
			25	25		
7	C	21	Total	O	0	0
			21	21		

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.

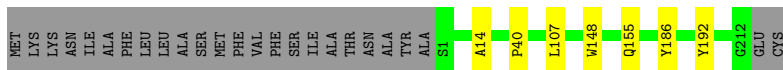
- Molecule 1: anti-CD16a Fab light chain

Chain L: 



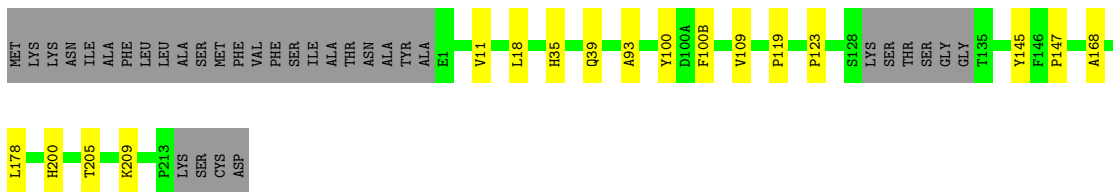
- Molecule 1: anti-CD16a Fab light chain

Chain B: 



- Molecule 2: anti-CD16A Fab heavy chain

Chain H: 



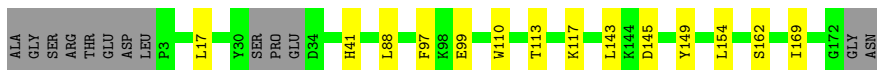
- Molecule 2: anti-CD16A Fab heavy chain

Chain A: 



- Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain D: 



● Molecule 3: Low affinity immunoglobulin gamma Fc region receptor III-A

Chain C:

88%

5%

7%



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

Chain E:

50%

50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.31Å 220.56Å 70.83Å 90.00° 108.55° 90.00°	Depositor
Resolution (Å)	33.88 – 2.16 33.88 – 2.16	Depositor EDS
% Data completeness (in resolution range)	91.8 (33.88-2.16) 91.8 (33.88-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	62.14 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.189 , 0.234 0.190 , 0.236	Depositor DCC
R_{free} test set	3164 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.286 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.330 for -h,-k,h+l	Depositor
Outliers	0 of 64736 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	B	0.09	0/1634	0.30	0/2228
1	L	0.09	0/1630	0.28	0/2223
2	A	0.09	0/1666	0.28	0/2271
2	H	0.10	0/1662	0.31	0/2266
3	C	0.09	0/1342	0.28	0/1827
3	D	0.12	0/1376	0.32	0/1871
All	All	0.10	0/9310	0.29	0/12686

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 [i](#)

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	B	1598	0	1526	3	0
1	L	1594	0	1522	8	0
2	A	1624	0	1553	6	0
2	H	1620	0	1550	11	0
3	C	1308	0	1222	6	0
3	D	1339	0	1249	12	0
4	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	6	0	8	0	0
6	C	28	0	26	0	0
6	D	14	0	13	0	0
7	A	48	0	0	0	0
7	B	31	0	0	0	0
7	C	21	0	0	1	0
7	D	25	0	0	0	0
7	H	50	0	0	1	0
7	L	23	0	0	0	0
All	All	9357	0	8694	45	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 45 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:H:168:ALA:HB2	2:H:178:LEU:HD23	1.76	0.66
2:A:119:PRO:HB3	2:A:145:TYR:HB3	1.81	0.63
3:C:41:HIS:NE2	3:C:63:SER:O	2.29	0.61
2:H:35:HIS:HB2	2:H:93:ALA:HB3	1.84	0.59
2:A:117:LYS:NZ	2:A:144:ASP:O	2.33	0.59

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	B	209/236 (89%)	198 (95%)	10 (5%)	1 (0%)	24 20
1	L	209/236 (89%)	201 (96%)	6 (3%)	2 (1%)	12 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	212/247 (86%)	208 (98%)	4 (2%)	0	100	100
2	H	211/247 (85%)	203 (96%)	8 (4%)	0	100	100
3	C	163/180 (91%)	157 (96%)	6 (4%)	0	100	100
3	D	164/180 (91%)	157 (96%)	7 (4%)	0	100	100
All	All	1168/1326 (88%)	1124 (96%)	41 (4%)	3 (0%)	36	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	76	SER
1	L	77	GLY
1	B	40	PRO

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	B	180/203 (89%)	180 (100%)	0	100	100
1	L	179/203 (88%)	178 (99%)	1 (1%)	78	84
2	A	176/208 (85%)	176 (100%)	0	100	100
2	H	178/208 (86%)	178 (100%)	0	100	100
3	C	139/160 (87%)	139 (100%)	0	100	100
3	D	144/160 (90%)	144 (100%)	0	100	100
All	All	996/1142 (87%)	995 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	12	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	164	HIS
2	A	199	ASN
2	H	171	GLN
1	B	137	ASN
1	B	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	1	3,4	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.43	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
4	NAG	E	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

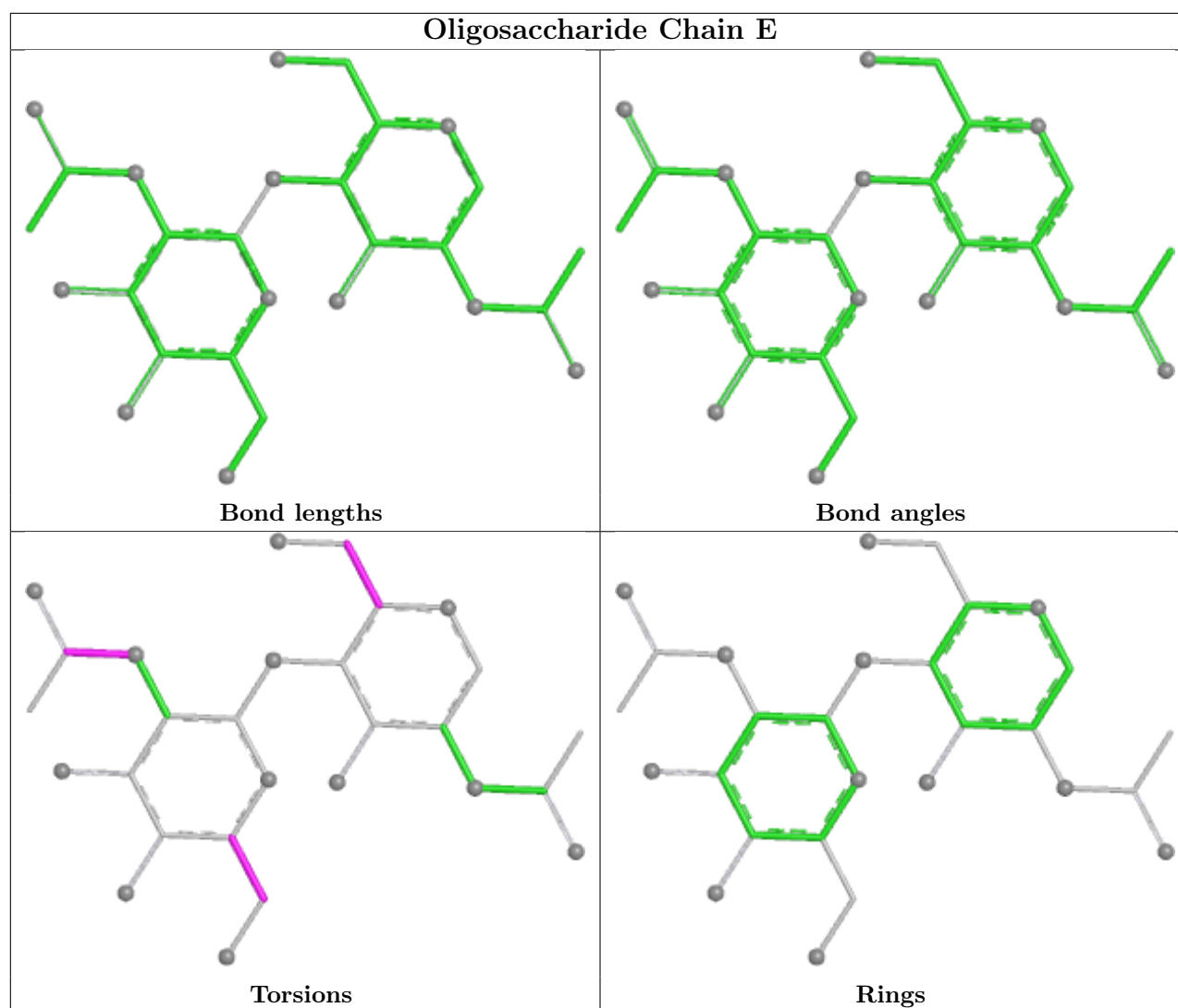
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	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](#)

4 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	NAG	C	201	3	14,14,15	0.20	0	17,19,21	0.41	0
6	NAG	C	202	-	14,14,15	0.22	0	17,19,21	0.44	0
5	GOL	L	301	-	5,5,5	0.91	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	201	3	14,14,15	0.20	0	17,19,21	0.46	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	NAG	C	201	3	-	2/6/23/26	0/1/1/1
6	NAG	C	202	-	-	4/6/23/26	0/1/1/1
5	GOL	L	301	-	-	2/4/4/4	-
6	NAG	D	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	NAG	O5-C5-C6-O6
6	C	201	NAG	C4-C5-C6-O6
6	C	202	NAG	C8-C7-N2-C2
6	C	202	NAG	O7-C7-N2-C2
6	C	202	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	211/236 (89%)	-0.79	0 100 100	33, 48, 73, 113	0
1	L	211/236 (89%)	-0.74	0 100 100	34, 47, 67, 94	0
2	A	216/247 (87%)	-0.90	0 100 100	30, 41, 59, 82	0
2	H	214/247 (86%)	-0.89	0 100 100	21, 40, 57, 80	1 (0%)
3	C	167/180 (92%)	-0.64	0 100 100	35, 55, 83, 154	0
3	D	167/180 (92%)	-0.65	0 100 100	21, 52, 82, 129	1 (0%)
All	All	1186/1326 (89%)	-0.78	0 100 100	21, 46, 73, 154	2 (0%)

There are no RSRZ outliers to report.

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

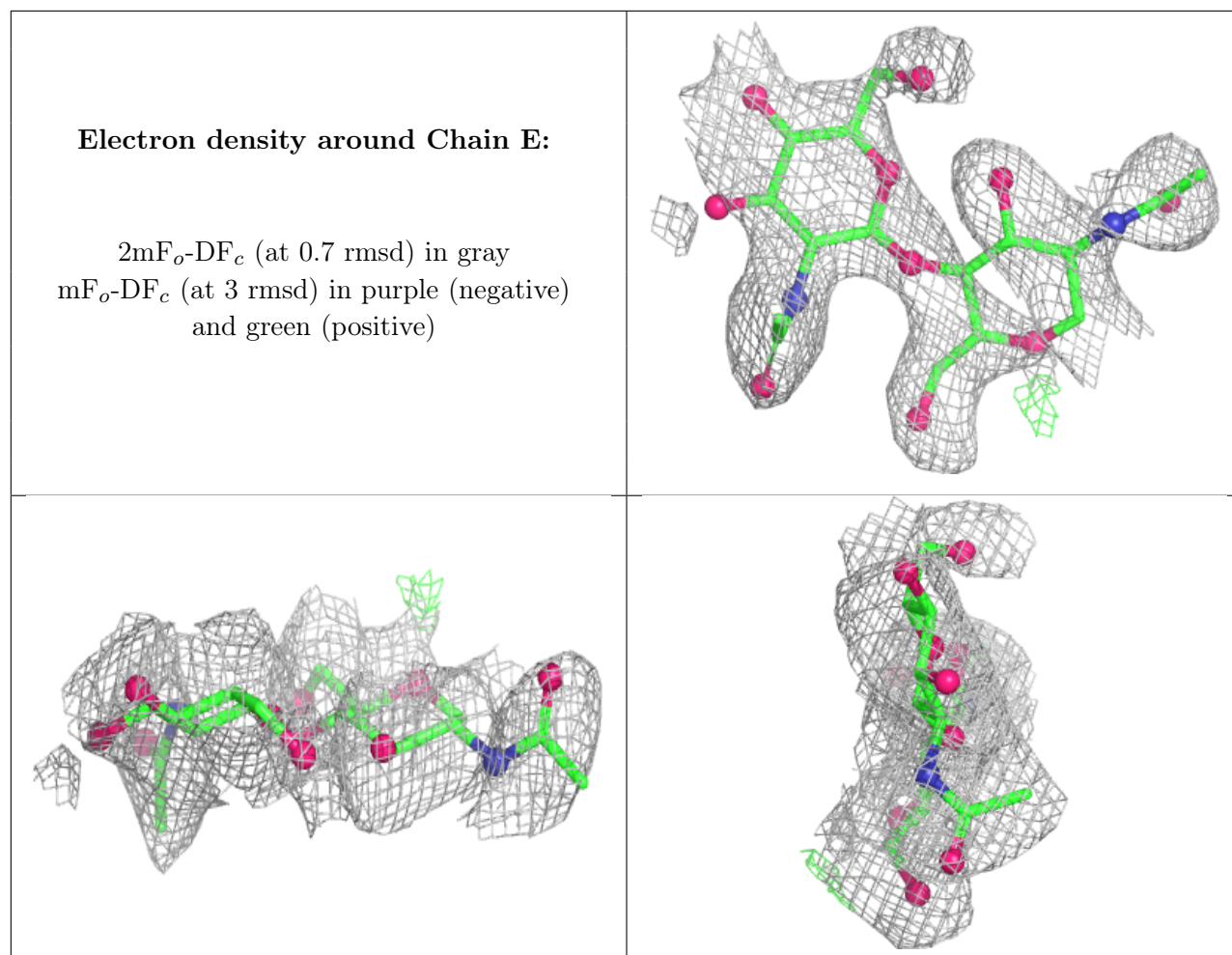
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	NAG	E	1	14/15	-	-	45,54,61,64	0
4	NAG	E	2	14/15	-	-	50,66,70,73	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, 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	NAG	C	202	14/15	0.96	0.07	47,63,74,81	0
6	NAG	D	201	14/15	0.97	0.06	41,53,63,67	0
6	NAG	C	201	14/15	0.97	0.05	53,57,65,69	0
5	GOL	L	301	6/6	0.97	0.07	40,56,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.