



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:29 PM UTC

PDB ID : 8A47 / pdb\_00008a47  
Title : IdeS in complex with IgG1 Fc  
Authors : Sudol, A.S.L.; Tews, I.; Crispin, M.  
Deposited on : 2022-06-10  
Resolution : 2.34 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](mailto: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)  
Xtrriage (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

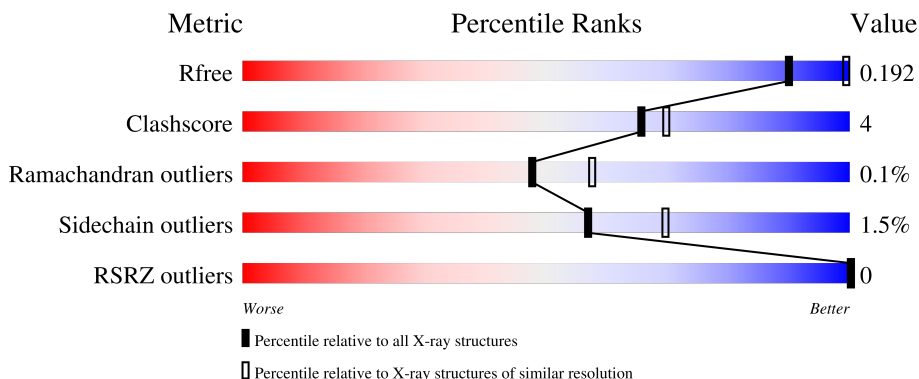
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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	A	227	89% (Green), 6% (Yellow), 5% (Grey)
1	B	227	88% (Green), 7% (Yellow), 5% (Grey)
2	C	308	80% (Green), 16% (Yellow), 4% (Grey)
3	D	7	71% (Green), 29% (Yellow)
4	E	8	100% (Green)

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12063 atoms, of which 5878 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 IgG1 Fc.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	217	3435	1102	1704	290	331	8	107	1	0
1	B	215	3396	1089	1687	287	326	7	106	0	0

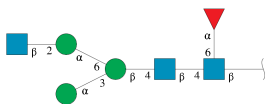
- Molecule 2 is a protein called IgG-degrading protease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	297	4674	1501	2314	402	452	5	145	0	0

There are 10 discrepancies between the modelled and reference sequences:

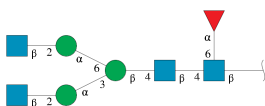
Chain	Residue	Modelled	Actual	Comment	Reference
C	40	MET	-	initiating methionine	UNP A0A8B6IYA1
C	94	ALA	CYS	engineered mutation	UNP A0A8B6IYA1
C	350	LEU	-	expression tag	UNP A0A8B6IYA1
C	351	GLU	-	expression tag	UNP A0A8B6IYA1
C	352	HIS	-	expression tag	UNP A0A8B6IYA1
C	353	HIS	-	expression tag	UNP A0A8B6IYA1
C	354	HIS	-	expression tag	UNP A0A8B6IYA1
C	355	HIS	-	expression tag	UNP A0A8B6IYA1
C	356	HIS	-	expression tag	UNP A0A8B6IYA1
C	357	HIS	-	expression tag	UNP A0A8B6IYA1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	7	Total	C	H	N	O	18	0	0
			165	48	80	3	34			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	8	Total	C	H	N	O	20	0	0
			192	56	93	4	39			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	65	Total	O	0	0
			65	65		
6	C	90	Total	O	0	0
			90	90		

### 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.

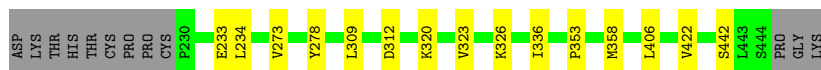
- Molecule 1: IgG1 Fc

Chain A:  89% 6%




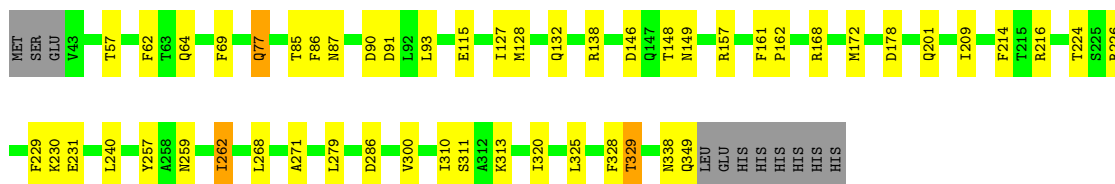
- Molecule 1: IgG1 Fc

Chain B:  88% 7% 5%



- Molecule 2: IgG-degrading protease

Chain C:  80% 16%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  71% 29%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1  
MAG2  
BKA3  
MAN4  
MAG5  
MAG6  
MAG7  
FUC8

## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.56Å 108.45Å 63.09Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	48.53 – 2.34 48.53 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.53-2.34) 95.2 (48.53-2.34)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.171 , 0.203 0.161 , 0.192	Depositor DCC
$R_{free}$ test set	3049 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 18.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.427 for -h,-k,l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for -h,-k,l	Depositor
Outliers	0 of 60351 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, BMA, FUC, MAN, NA

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	0.56	0/1780	0.93	0/2427
1	B	0.61	0/1757	0.96	0/2394
2	C	0.58	0/2412	1.09	2/3263 (0.1%)
All	All	0.58	0/5949	1.01	2/8084 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	214	PHE	CA-CB-CG	-5.50	108.30	113.80
2	C	286	ASP	CA-CB-CG	5.46	118.06	112.60

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	A	1731	1704	1696	9	1
1	B	1709	1687	1680	7	1
2	C	2360	2314	2303	30	0
3	D	85	80	73	0	0
4	E	99	93	85	0	0
5	C	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	45	0	0	3	0
6	B	65	0	0	2	0
6	C	90	0	0	3	0
All	All	6185	5878	5837	45	1

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 4.

All (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:C:62:PHE:HB3	2:C:69:PHE:CZ	2.31	0.65
2:C:64:GLN:NE2	6:C:501:HOH:O	2.20	0.64
1:B:422:VAL:HG22	1:B:442:SER:HB2	1.81	0.63
2:C:271:ALA:HB1	2:C:279:LEU:HD21	1.79	0.63
2:C:57:THR:HB	2:C:77:GLN:HG3	1.82	0.61
1:A:247:PRO:HB3	1:A:376:ASP:HB3	1.83	0.59
6:B:532:HOH:O	2:C:162:PRO:HG2	2.03	0.59
2:C:87:ASN:HD21	2:C:157:ARG:HD2	1.67	0.57
2:C:127:ILE:HD11	2:C:209:ILE:HD11	1.87	0.57
1:A:388:GLU:OE2	1:A:416:ARG:NH2	2.38	0.57
1:B:406:LEU:HD12	1:B:406:LEU:C	2.33	0.53
2:C:311:SER:HB3	2:C:313:LYS:O	2.09	0.53
1:A:406:LEU:C	1:A:406:LEU:HD12	2.35	0.52
2:C:201:GLN:O	2:C:216:ARG:NH1	2.43	0.52
2:C:128:MET:HE3	2:C:132:GLN:O	2.10	0.51
1:A:309:LEU:HB2	1:A:312:ASP:OD2	2.10	0.51
1:B:326:LYS:HG2	6:B:513:HOH:O	2.11	0.50
2:C:230:LYS:O	2:C:231:GLU:HB2	2.12	0.50
2:C:226:ARG:HG3	2:C:328:PHE:CE2	2.47	0.50
2:C:127:ILE:HD11	2:C:209:ILE:CD1	2.42	0.49
2:C:161:PHE:N	2:C:162:PRO:CD	2.77	0.47
6:A:525:HOH:O	2:C:172:MET:CE	2.63	0.46
2:C:90:ASP:HA	2:C:93:LEU:HD12	1.98	0.46
2:C:329:THR:HG22	6:C:566:HOH:O	2.15	0.45
2:C:146:ASP:OD1	2:C:149:ASN:N	2.48	0.45
1:B:278:TYR:HB2	1:B:320:LYS:HB3	1.99	0.45
2:C:115:GLU:CD	2:C:138:ARG:HH22	2.25	0.45
1:B:309:LEU:HB2	1:B:312:ASP:OD2	2.16	0.45
2:C:268:LEU:C	2:C:268:LEU:HD23	2.42	0.44
1:A:278:TYR:HB2	1:A:320:LYS:HB3	2.00	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:ASN:ND2	2:C:262:ILE:O	2.43	0.44
1:A:355:ARG:NH1	6:A:511:HOH:O	2.51	0.44
1:B:353:PRO:HB2	1:B:358:MET:HE3	2.00	0.44
1:B:273:VAL:HG13	1:B:323:VAL:HG13	2.00	0.43
2:C:271:ALA:HB1	2:C:279:LEU:CD2	2.45	0.43
1:A:388:GLU:CD	1:A:416:ARG:HH22	2.27	0.43
2:C:85:THR:O	2:C:86:PHE:HB2	2.18	0.42
6:A:525:HOH:O	2:C:172:MET:HE2	2.18	0.42
2:C:229:PHE:HE1	2:C:240:LEU:HD23	1.85	0.42
2:C:338:ASN:O	2:C:349:GLN:HB2	2.19	0.42
2:C:178:ASP:OD1	2:C:224:THR:OG1	2.30	0.42
1:A:233:GLU:HG3	2:C:325:LEU:HD13	2.02	0.41
2:C:90:ASP:O	2:C:91:ASP:C	2.63	0.41
1:A:232:PRO:HB2	6:C:564:HOH:O	2.21	0.41
2:C:300:VAL:HG22	2:C:310:ILE:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:HH11	1:B:233:GLU:OE2[4_555]	1.58	0.02

## 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	216/227 (95%)	213 (99%)	2 (1%)	1 (0%)	24 26
1	B	213/227 (94%)	211 (99%)	2 (1%)	0	100 100
2	C	295/308 (96%)	280 (95%)	15 (5%)	0	100 100
All	All	724/762 (95%)	704 (97%)	19 (3%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	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	A	201/209 (96%)	199 (99%)	2 (1%)	68	79
1	B	198/209 (95%)	196 (99%)	2 (1%)	68	79
2	C	252/264 (96%)	245 (97%)	7 (3%)	38	50
All	All	651/682 (96%)	640 (98%)	11 (2%)	57	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	356[A]	GLU
1	A	356[B]	GLU
1	B	234	LEU
1	B	336	ILE
2	C	77	GLN
2	C	148	THR
2	C	168	ARG
2	C	257	TYR
2	C	262	ILE
2	C	320	ILE
2	C	329	THR

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

15 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
3	NAG	D	1	1,3	14,14,15	0.86	0	17,19,21	1.03	0
3	NAG	D	2	3	14,14,15	1.19	1 (7%)	17,19,21	0.60	0
3	BMA	D	3	3	11,11,12	0.93	0	15,15,17	0.75	0
3	MAN	D	4	3	11,11,12	0.93	0	15,15,17	0.93	0
3	NAG	D	5	3	14,14,15	0.87	0	17,19,21	1.04	1 (5%)
3	MAN	D	6	3	11,11,12	0.62	0	15,15,17	0.54	0
3	FUC	D	7	3	10,10,11	1.01	0	14,14,16	0.99	0
4	NAG	E	1	4,1	14,14,15	0.89	0	17,19,21	0.73	0
4	NAG	E	2	4	14,14,15	0.58	0	17,19,21	0.60	0
4	BMA	E	3	4	11,11,12	0.75	0	15,15,17	0.83	0
4	MAN	E	4	4	11,11,12	0.94	0	15,15,17	0.74	0
4	NAG	E	5	4	14,14,15	0.62	0	17,19,21	0.76	0
4	MAN	E	6	4	11,11,12	1.05	0	15,15,17	1.01	0
4	NAG	E	7	4	14,14,15	0.71	0	17,19,21	0.83	0
4	FUC	E	8	4	10,10,11	0.67	0	14,14,16	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	MAN	D	6	3	-	1/2/19/22	0/1/1/1
3	FUC	D	7	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	NAG	E	5	4	-	0/6/23/26	0/1/1/1
4	MAN	E	6	4	-	1/2/19/22	0/1/1/1
4	NAG	E	7	4	-	0/6/23/26	0/1/1/1
4	FUC	E	8	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C4-C5	2.19	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	NAG	C6-C5-C4	2.26	118.57	113.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

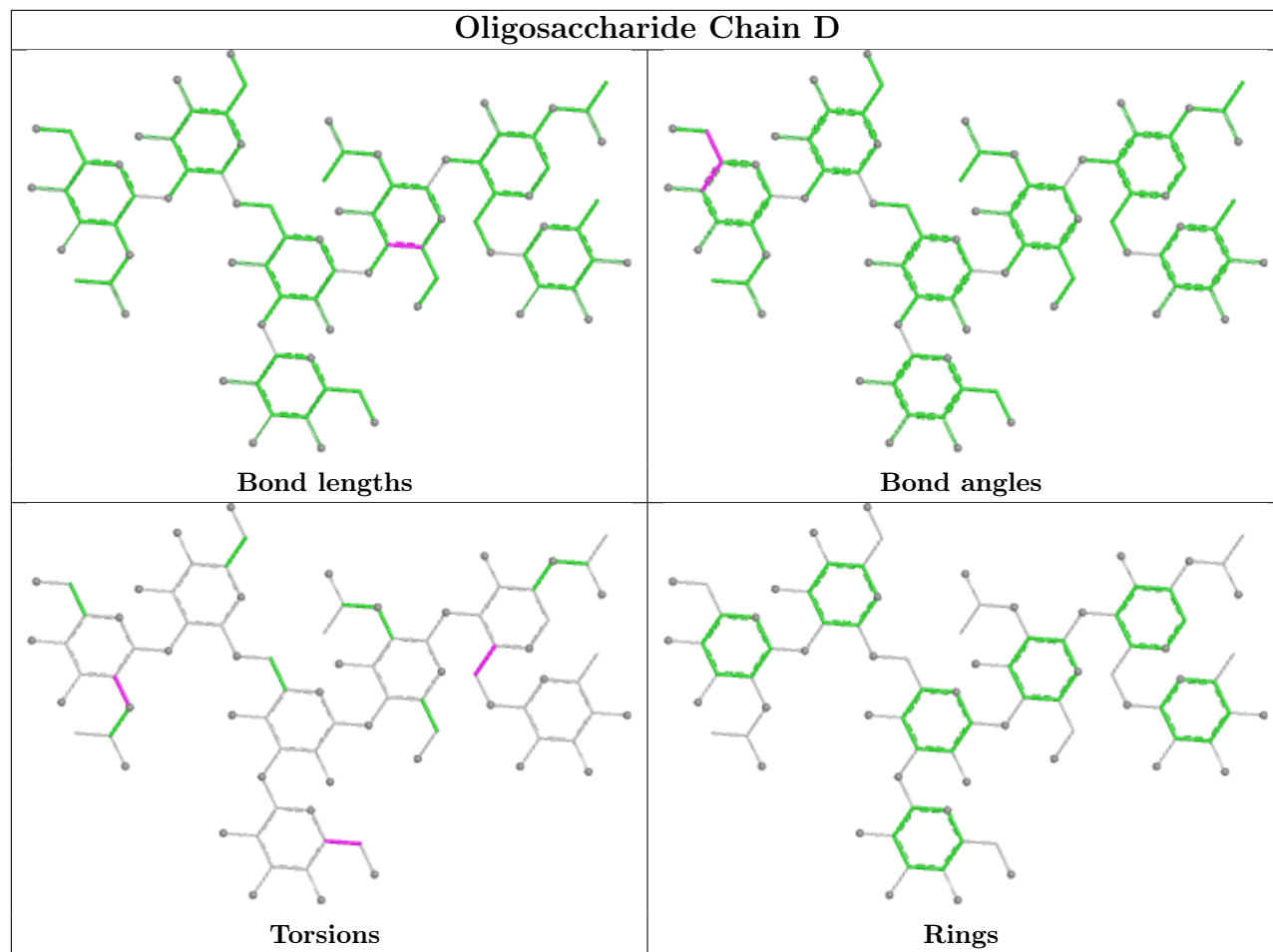
Mol	Chain	Res	Type	Atoms
4	E	4	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	D	5	NAG	C3-C2-N2-C7
3	D	6	MAN	O5-C5-C6-O6
3	D	5	NAG	C1-C2-N2-C7

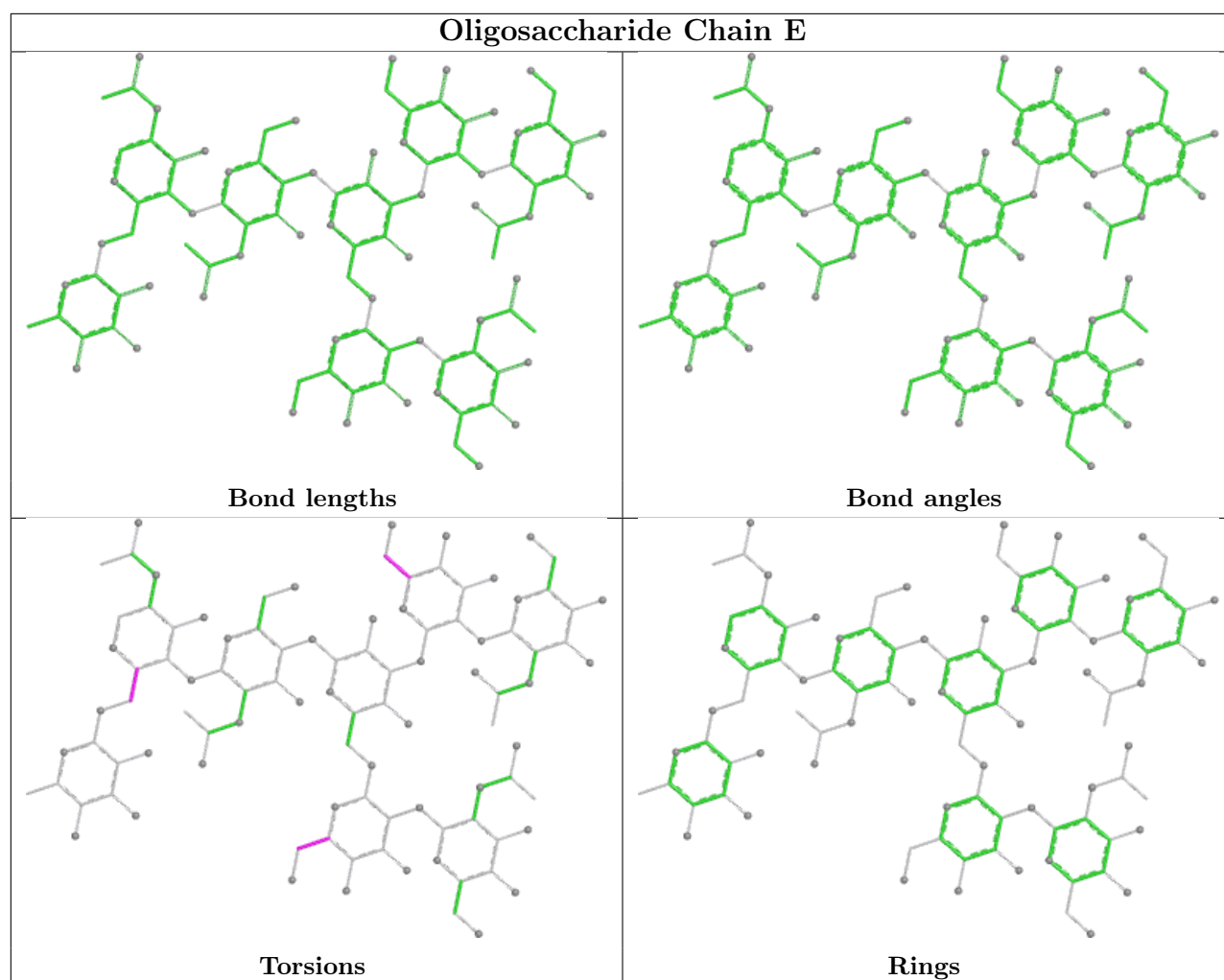
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	217/227 (95%)	-1.54	0 100 100	19, 41, 68, 86	1 (0%)
1	B	215/227 (94%)	-1.66	0 100 100	20, 31, 48, 75	0
2	C	297/308 (96%)	-1.65	0 100 100	18, 34, 54, 84	0
All	All	729/762 (95%)	-1.62	0 100 100	18, 35, 61, 86	1 (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, 95<sup>th</sup> 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.

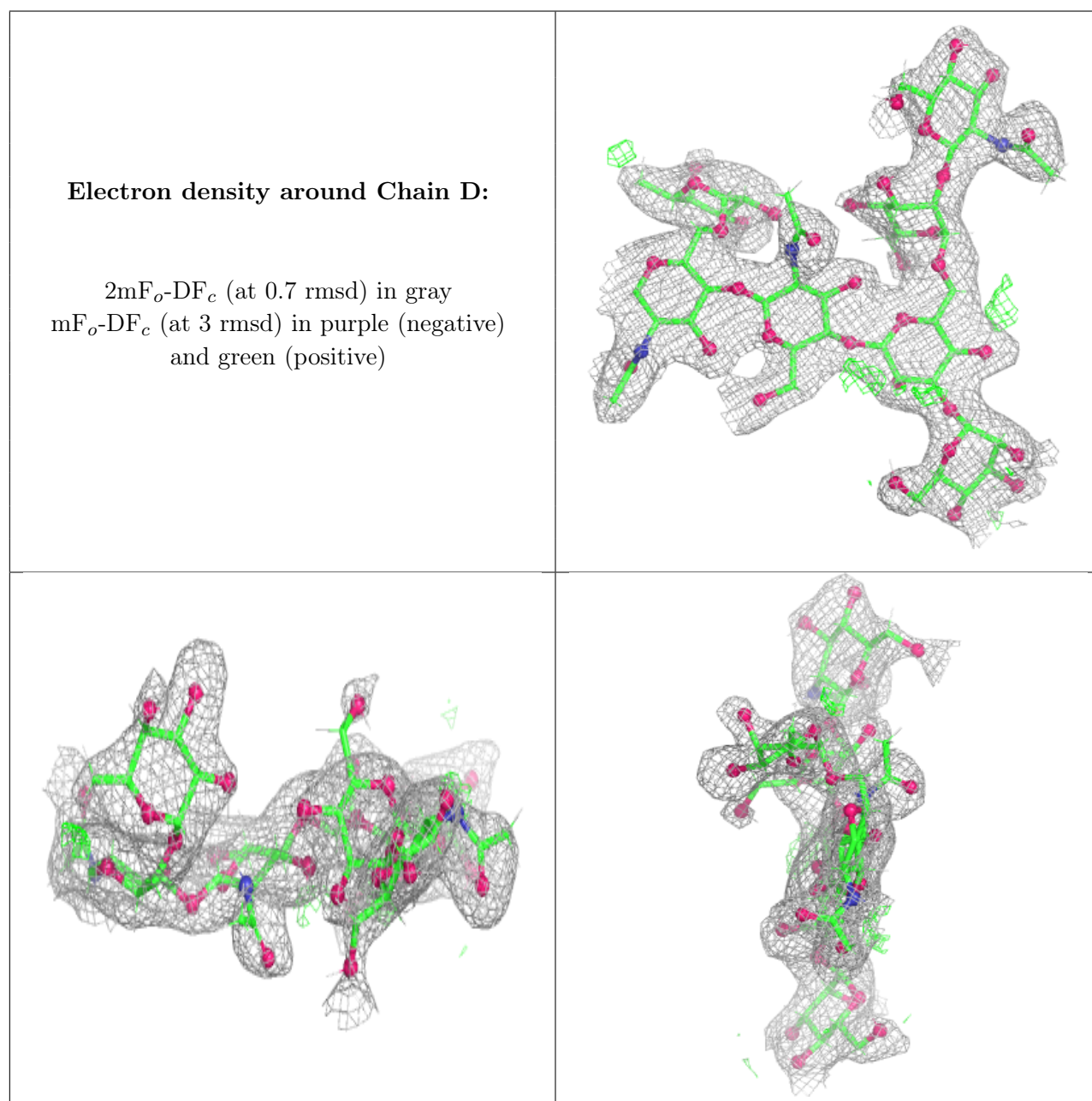
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	2	14/15	0.99	0.04	40,56,63,68	2
3	BMA	D	3	11/12	0.99	0.03	40,47,50,50	2
3	MAN	D	4	11/12	0.99	0.04	42,50,58,63	3
3	NAG	D	5	14/15	0.99	0.04	46,56,60,60	3
3	MAN	D	6	11/12	0.99	0.04	41,52,58,59	4
3	FUC	D	7	10/11	0.99	0.04	43,54,57,60	3
4	MAN	E	4	11/12	0.99	0.03	36,43,48,50	3
4	NAG	E	5	14/15	0.99	0.04	39,55,67,70	3
4	MAN	E	6	11/12	0.99	0.02	31,34,37,37	3
4	BMA	E	3	11/12	1.00	0.02	29,34,37,39	2

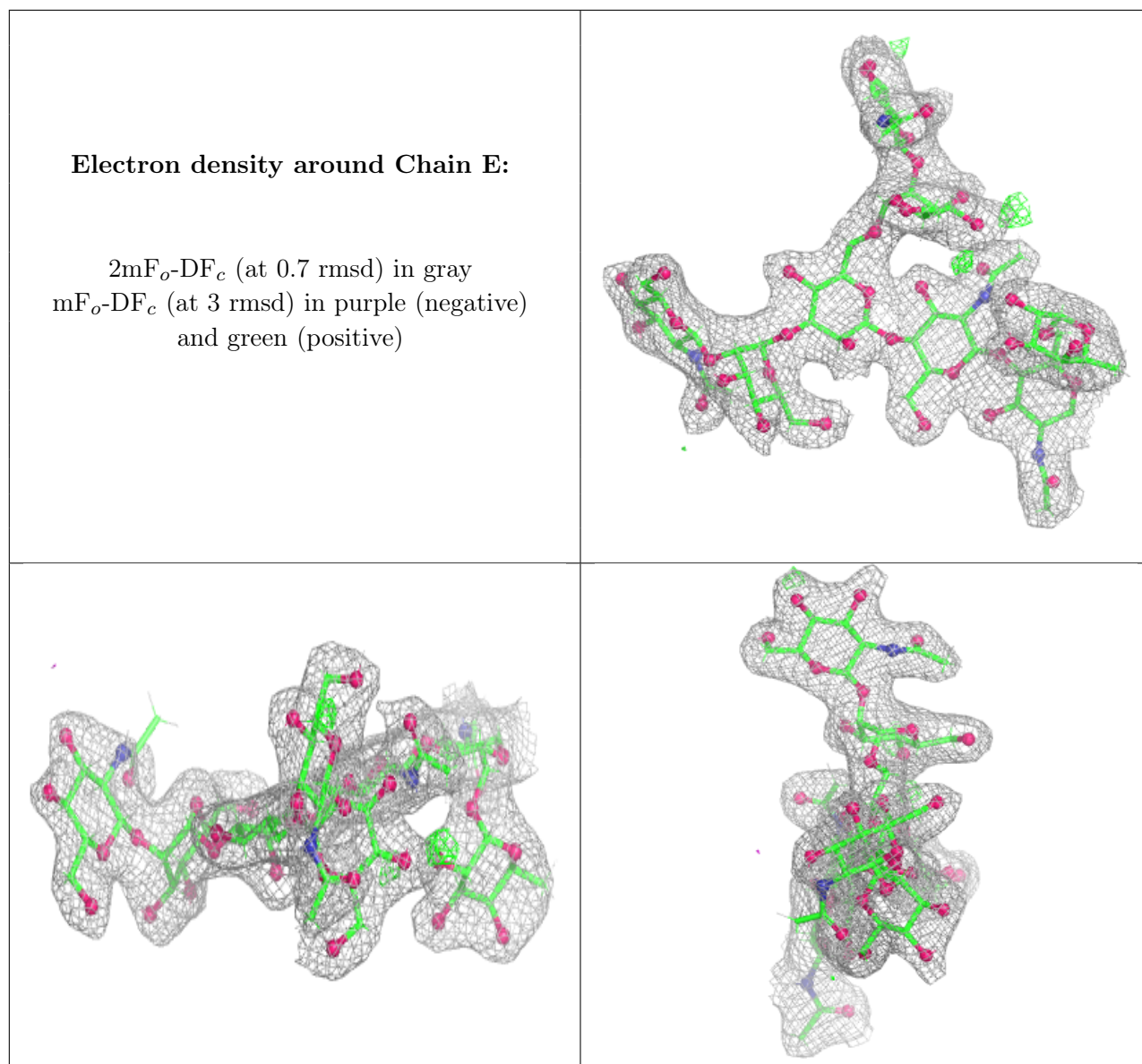
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1	14/15	1.00	0.03	39,48,53,56	1
4	NAG	E	1	14/15	1.00	0.01	27,29,31,35	1
4	NAG	E	2	14/15	1.00	0.02	29,31,33,34	2
4	NAG	E	7	14/15	1.00	0.02	31,36,43,45	3
4	FUC	E	8	10/11	1.00	0.03	35,43,48,48	3

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NA	C	401	1/1	1.00	0.02	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.