



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:28 PM UTC

PDB ID : 8A49 / pdb_00008a49
Title : Endoglycosidase S in complex with IgG1 Fc
Authors : Sudol, A.S.L.; Tews, I.; Crispin, M.
Deposited on : 2022-06-10
Resolution : 3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

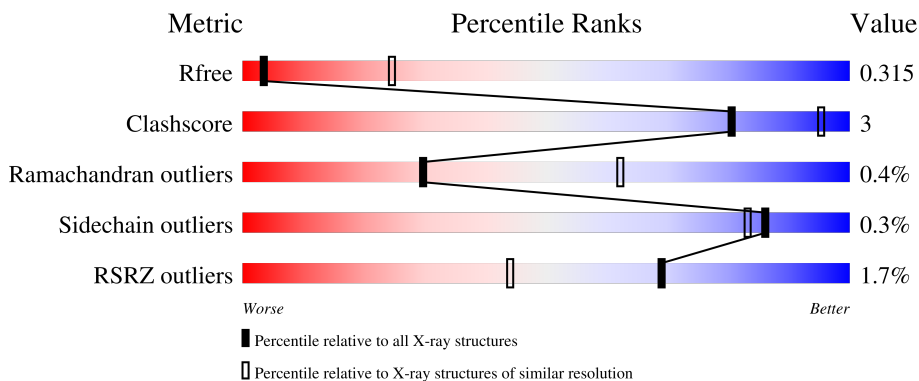
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	A	227	 83% 8% 9%
1	B	227	 81% 10% 9%
2	C	906	 91% 7% .
2	D	906	 91% 6% .
3	E	8	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 33731 atoms, of which 16644 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	207	3265	1048	1618	279	313	7	110	0	0
1	B	207	3224	1035	1601	276	305	7	113	0	0

- Molecule 2 is a protein called Secreted endoglycosidase EndoS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	884	13643	4361	6754	1150	1362	16	422	0	0
2	D	879	13339	4270	6578	1133	1342	16	428	0	0

There are 24 discrepancies between the modelled and reference sequences:

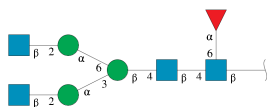
Chain	Residue	Modelled	Actual	Comment	Reference
C	99	MET	-	initiating methionine	UNP Q9APG4
C	233	ALA	ASP	engineered mutation	UNP Q9APG4
C	235	LEU	GLU	engineered mutation	UNP Q9APG4
C	996	LEU	-	expression tag	UNP Q9APG4
C	997	LEU	-	expression tag	UNP Q9APG4
C	998	GLU	-	expression tag	UNP Q9APG4
C	999	HIS	-	expression tag	UNP Q9APG4
C	1000	HIS	-	expression tag	UNP Q9APG4
C	1001	HIS	-	expression tag	UNP Q9APG4
C	1002	HIS	-	expression tag	UNP Q9APG4
C	1003	HIS	-	expression tag	UNP Q9APG4
C	1004	HIS	-	expression tag	UNP Q9APG4
D	99	MET	-	initiating methionine	UNP Q9APG4
D	233	ALA	ASP	engineered mutation	UNP Q9APG4
D	235	LEU	GLU	engineered mutation	UNP Q9APG4
D	996	LEU	-	expression tag	UNP Q9APG4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	997	LEU	-	expression tag	UNP Q9APG4
D	998	GLU	-	expression tag	UNP Q9APG4
D	999	HIS	-	expression tag	UNP Q9APG4
D	1000	HIS	-	expression tag	UNP Q9APG4
D	1001	HIS	-	expression tag	UNP Q9APG4
D	1002	HIS	-	expression tag	UNP Q9APG4
D	1003	HIS	-	expression tag	UNP Q9APG4
D	1004	HIS	-	expression tag	UNP Q9APG4

- Molecule 3 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	
			Total	C	H	N				O
3	E	8	192	56	93	4	39	20	0	0

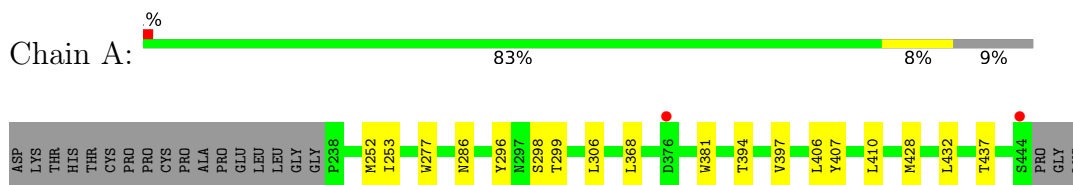
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	C	31	Total	O	0	0
			31	31		
4	D	17	Total	O	0	0
			17	17		
4	B	14	Total	O	0	0
			14	14		

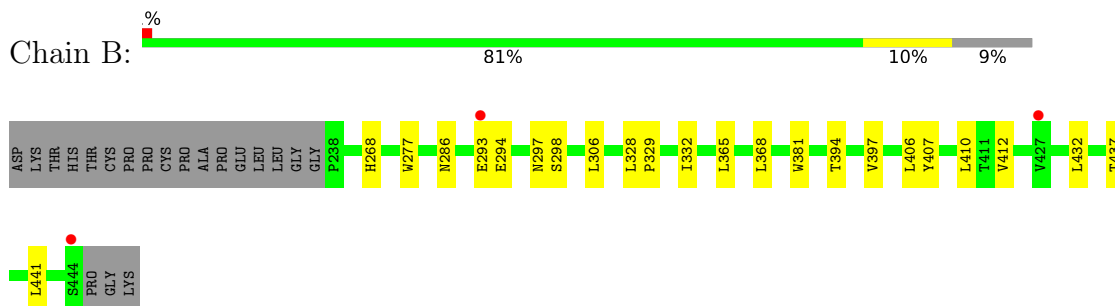
3 Residue-property plots [i](#)

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.

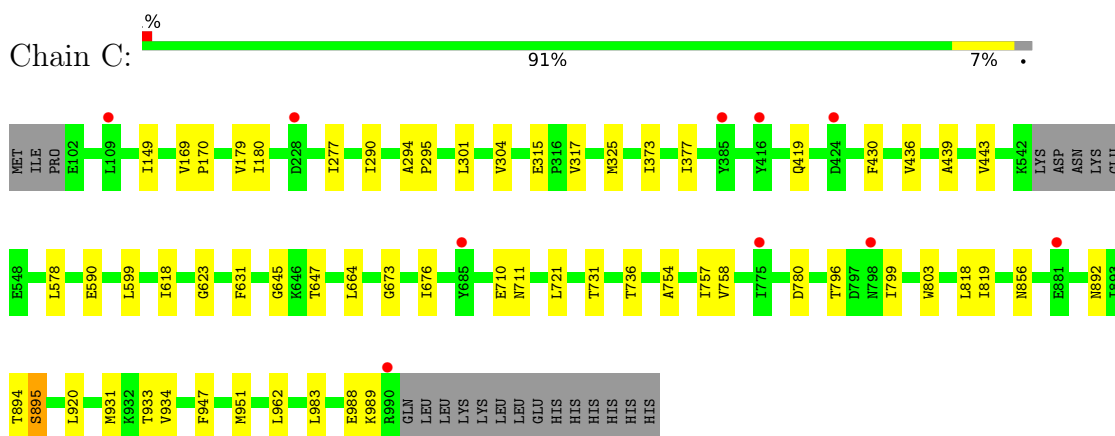
- Molecule 1: IgG1 Fc



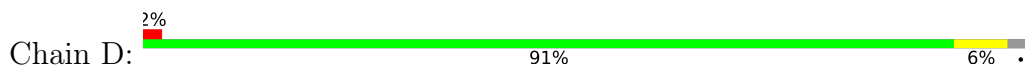
- Molecule 1: IgG1 Fc

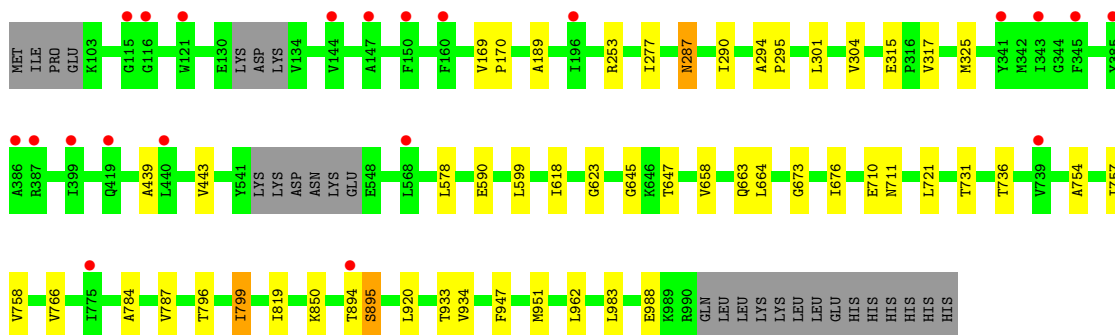


- Molecule 2: Secreted endoglycosidase EndoS



- Molecule 2: Secreted endoglycosidase EndoS





- Molecule 3: 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
MAG3
MAN4
MAG5
MAN6
MAG7
FUC8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.53Å 174.29Å 193.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 3.45 49.78 – 3.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.78-3.45) 93.5 (49.78-3.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.253 , 0.311 0.258 , 0.315	Depositor DCC
R_{free} test set	2118 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	116.4	Xtrriage
Anisotropy	0.278	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 97.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33731	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: MAN, BMA, FUC, 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	0.45	0/1693	0.69	0/2308
1	B	0.46	0/1668	0.70	0/2275
2	C	0.43	0/7031	0.76	0/9538
2	D	0.43	0/6898	0.77	0/9368
All	All	0.43	0/17290	0.75	0/23489

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	A	1647	1618	1603	11	0
1	B	1623	1601	1575	14	0
2	C	6889	6754	6676	37	1
2	D	6761	6578	6463	32	1
3	E	99	93	85	0	0
4	A	6	0	0	0	0
4	B	14	0	0	0	0
4	C	31	0	0	0	0
4	D	17	0	0	1	0
All	All	17087	16644	16402	87	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 3.

All (87) 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:796:THR:HG22	1:B:286:ASN:HD22	1.42	0.83
2:C:304:VAL:HG21	2:C:325:MET:HE1	1.70	0.73
2:D:304:VAL:HG21	2:D:325:MET:HE1	1.69	0.73
1:A:286:ASN:HD22	2:C:796:THR:HG22	1.53	0.71
2:D:294:ALA:HB3	2:D:295:PRO:HD3	1.79	0.63
2:C:294:ALA:HB3	2:C:295:PRO:HD3	1.80	0.62
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.81	0.62
2:C:180:ILE:HD13	2:C:277:ILE:HD12	1.83	0.61
2:C:818:LEU:HD11	2:C:931:MET:HE2	1.85	0.57
1:A:253:ILE:HD11	2:C:780:ASP:HB2	1.87	0.56
1:A:253:ILE:HG23	2:C:803:TRP:CZ2	2.42	0.55
2:D:799:ILE:HD12	2:D:799:ILE:N	2.22	0.55
1:A:381:TRP:CE3	1:A:410:LEU:HD22	2.43	0.54
1:B:381:TRP:CE3	1:B:410:LEU:HD22	2.43	0.54
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.43	0.53
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.43	0.53
2:C:894:THR:O	2:C:895:SER:C	2.51	0.53
2:D:304:VAL:CG2	2:D:325:MET:HE1	2.39	0.53
1:A:432:LEU:HD13	1:A:437:THR:HG22	1.91	0.52
2:D:894:THR:O	2:D:895:SER:C	2.51	0.52
1:B:432:LEU:HD13	1:B:437:THR:HG22	1.92	0.52
2:D:189:ALA:HB1	2:D:253:ARG:HE	1.73	0.52
2:C:373:ILE:HD11	2:C:430:PHE:CD2	2.46	0.51
2:C:373:ILE:HD11	2:C:430:PHE:CG	2.46	0.51
2:C:304:VAL:CG2	2:C:325:MET:HE1	2.40	0.51
2:C:315:GLU:OE1	2:C:317:VAL:HG22	2.11	0.51
2:D:439:ALA:O	2:D:443:VAL:HG23	2.12	0.50
2:C:892:ASN:HB3	2:C:931:MET:HE2	1.93	0.49
2:D:315:GLU:OE2	2:D:317:VAL:HG22	2.12	0.49
2:D:933:THR:HG22	2:D:983:LEU:HD23	1.93	0.49
2:C:439:ALA:O	2:C:443:VAL:HG23	2.12	0.49
2:D:277:ILE:CG2	2:D:301:LEU:HD13	2.43	0.49
2:C:933:THR:HG22	2:C:983:LEU:HD23	1.95	0.49
2:C:277:ILE:CG2	2:C:301:LEU:HD13	2.44	0.48
2:C:664:LEU:HD13	2:C:754:ALA:CB	2.43	0.48
2:C:736:THR:HG23	2:C:757:ILE:HG12	1.96	0.48
2:D:664:LEU:HD13	2:D:754:ALA:CB	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLU:O	1:B:294:GLU:C	2.56	0.48
2:D:766:VAL:HG12	4:D:1116:HOH:O	2.14	0.47
2:C:721:LEU:HD12	2:C:920:LEU:HD22	1.96	0.46
2:D:736:THR:HG23	2:D:757:ILE:HG12	1.97	0.46
2:D:676:ILE:HD12	2:D:676:ILE:N	2.31	0.46
2:C:676:ILE:HD12	2:C:676:ILE:N	2.32	0.45
1:B:365:LEU:HD13	1:B:412:VAL:HG22	1.97	0.45
2:D:721:LEU:HD12	2:D:920:LEU:HD22	1.98	0.45
2:D:934:VAL:HG22	2:D:962:LEU:HD23	1.99	0.45
2:C:934:VAL:HG22	2:C:962:LEU:HD23	1.98	0.44
1:B:365:LEU:HD23	1:B:441:LEU:HD23	1.98	0.44
2:D:658:VAL:CG1	2:D:663:GLN:HG3	2.47	0.44
1:B:406:LEU:HD12	1:B:406:LEU:C	2.43	0.43
2:C:290:ILE:O	2:C:294:ALA:HB2	2.19	0.43
2:C:731:THR:HG22	2:C:758:VAL:HG11	2.00	0.43
2:C:947:PHE:CD1	2:C:951:MET:HB2	2.54	0.43
2:D:287:ASN:HD21	2:D:290:ILE:HB	1.83	0.43
2:D:169:VAL:HB	2:D:170:PRO:HD3	2.01	0.43
1:B:277:TRP:CE3	1:B:306:LEU:HD22	2.53	0.43
1:A:406:LEU:C	1:A:406:LEU:HD12	2.43	0.43
2:D:590:GLU:O	2:D:618:ILE:HG23	2.18	0.43
2:C:710:GLU:O	2:C:711:ASN:HB2	2.19	0.43
2:C:590:GLU:O	2:C:618:ILE:HG23	2.18	0.43
2:D:731:THR:HG22	2:D:758:VAL:HG11	2.00	0.42
2:D:819:ILE:HD12	2:D:819:ILE:N	2.34	0.42
1:A:277:TRP:CE3	1:A:306:LEU:HD22	2.55	0.42
2:D:947:PHE:CD1	2:D:951:MET:HB3	2.54	0.42
2:C:169:VAL:HB	2:C:170:PRO:HD3	2.01	0.42
1:A:252:MET:HE3	1:A:428:MET:SD	2.60	0.42
2:C:149:ILE:HD11	2:C:179:VAL:CG1	2.50	0.42
2:D:710:GLU:O	2:D:711:ASN:HB2	2.19	0.42
1:A:397:VAL:HG21	1:B:394:THR:HA	2.01	0.42
1:A:394:THR:HA	1:B:397:VAL:HG21	2.02	0.42
2:C:819:ILE:HD12	2:C:819:ILE:N	2.35	0.41
2:C:419:GLN:HE22	1:B:329:PRO:HG2	1.86	0.41
2:D:618:ILE:HG22	2:D:623:GLY:O	2.21	0.41
2:C:377:ILE:HG22	2:C:436:VAL:HG13	2.02	0.41
2:C:578:LEU:HD21	2:C:599:LEU:CD1	2.51	0.41
2:C:988:GLU:O	2:C:989:LYS:CB	2.69	0.41
2:D:578:LEU:HD21	2:D:599:LEU:CD1	2.51	0.41
2:D:578:LEU:HD21	2:D:599:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:645:GLY:O	2:D:647:THR:HG23	2.21	0.41
2:D:799:ILE:HG22	2:D:799:ILE:O	2.21	0.41
2:C:645:GLY:O	2:C:647:THR:HG23	2.21	0.40
2:C:618:ILE:HG22	2:C:623:GLY:O	2.21	0.40
2:C:578:LEU:HD21	2:C:599:LEU:HD13	2.03	0.40
1:B:328:LEU:HA	1:B:329:PRO:HD3	1.95	0.40
2:C:799:ILE:O	2:C:799:ILE:HG22	2.22	0.40
2:D:290:ILE:O	2:D:294:ALA:HB2	2.21	0.40
2:D:784:ALA:O	2:D:787:VAL:HG22	2.22	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)
2:C:856:ASN:HD22	2:D:850:LYS:O[2_355]	1.39	0.21

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	205/227 (90%)	196 (96%)	8 (4%)	1 (0%)	24	57
1	B	205/227 (90%)	193 (94%)	10 (5%)	2 (1%)	12	44
2	C	880/906 (97%)	812 (92%)	65 (7%)	3 (0%)	36	67
2	D	873/906 (96%)	807 (92%)	64 (7%)	2 (0%)	43	74
All	All	2163/2266 (96%)	2008 (93%)	147 (7%)	8 (0%)	30	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	297	ASN
1	B	298	SER
2	C	895	SER
2	D	895	SER
2	C	631	PHE
2	C	673	GLY
2	D	673	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	190/210 (90%)	188 (99%)	2 (1%)	65	75
1	B	184/210 (88%)	183 (100%)	1 (0%)	81	81
2	C	738/792 (93%)	738 (100%)	0	100	100
2	D	711/792 (90%)	708 (100%)	3 (0%)	84	81
All	All	1823/2004 (91%)	1817 (100%)	6 (0%)	86	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	TYR
1	A	299	THR
2	D	287	ASN
2	D	799	ILE
2	D	988	GLU
1	B	268	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	ASN
1	A	362	GLN
1	A	384	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	390	ASN
1	A	418	GLN
1	A	421	ASN
1	A	434	ASN
2	C	122	HIS
2	C	173	ASN
2	C	287	ASN
2	C	351	ASN
2	C	353	GLN
2	C	412	GLN
2	C	671	ASN
2	C	672	GLN
2	C	686	GLN
2	C	798	ASN
2	C	807	GLN
2	C	836	ASN
2	D	151	HIS
2	D	173	ASN
2	D	210	ASN
2	D	287	ASN
2	D	351	ASN
2	D	353	GLN
2	D	362	ASN
2	D	412	GLN
2	D	671	ASN
2	D	686	GLN
2	D	687	ASN
2	D	807	GLN
1	B	286	ASN
1	B	384	ASN
1	B	418	GLN
1	B	421	ASN
1	B	434	ASN

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

8 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	E	1	1,3	14,14,15	0.38	0	17,19,21	0.87	0
3	NAG	E	2	3	14,14,15	0.30	0	17,19,21	0.62	0
3	BMA	E	3	3	11,11,12	0.28	0	15,15,17	0.53	0
3	MAN	E	4	3	11,11,12	0.26	0	15,15,17	0.67	0
3	NAG	E	5	3	14,14,15	0.24	0	17,19,21	0.43	0
3	MAN	E	6	3	11,11,12	0.27	0	15,15,17	0.52	0
3	NAG	E	7	3	14,14,15	0.33	0	17,19,21	0.50	0
3	FUC	E	8	3	10,10,11	0.30	0	14,14,16	0.67	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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	NAG	E	5	3	-	0/6/23/26	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	NAG	E	7	3	-	0/6/23/26	0/1/1/1
3	FUC	E	8	3	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

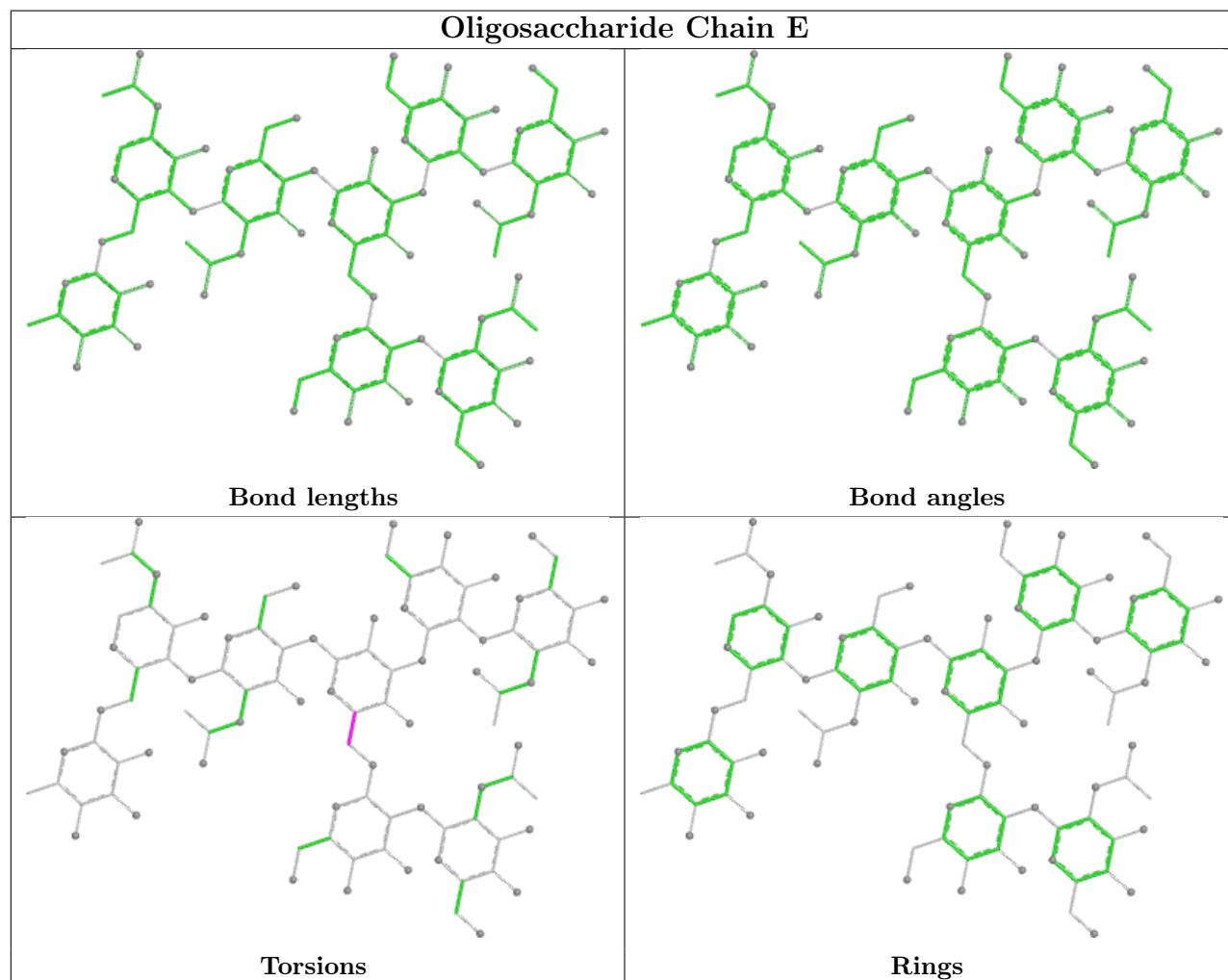
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6

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](#)

There are no ligands in this entry.

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

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	207/227 (91%)	-0.22	2 (0%) 79 56	90, 129, 165, 198	0
1	B	207/227 (91%)	-0.21	3 (1%) 73 49	91, 130, 180, 211	0
2	C	884/906 (97%)	-0.20	10 (1%) 78 54	93, 138, 176, 213	0
2	D	879/906 (97%)	-0.06	21 (2%) 59 37	109, 171, 224, 266	0
All	All	2177/2266 (96%)	-0.15	36 (1%) 69 44	90, 147, 211, 266	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	147	ALA	4.6
2	D	116	GLY	4.1
2	D	341	TYR	3.8
2	D	343	ILE	3.8
1	A	444	SER	3.4
2	D	386	ALA	3.2
2	D	399	ILE	3.0
1	B	427	VAL	3.0
2	D	419	GLN	3.0
2	D	440	LEU	2.7
2	D	144	VAL	2.7
2	D	739	VAL	2.7
2	D	160	PHE	2.5
2	C	990	ARG	2.4
2	C	385	TYR	2.4
1	B	444	SER	2.4
2	D	115	GLY	2.4
2	D	385	TYR	2.4
2	C	775	ILE	2.4
2	D	568	LEU	2.4
2	C	228	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	345	PHE	2.3
1	A	376	ASP	2.3
2	D	775	ILE	2.3
2	C	881	GLU	2.2
2	C	109	LEU	2.2
2	D	387	ARG	2.2
1	B	293	GLU	2.2
2	C	424	ASP	2.2
2	C	685	TYR	2.1
2	C	798	ASN	2.1
2	D	121	TRP	2.1
2	D	894	THR	2.1
2	D	150	PHE	2.0
2	D	196	ILE	2.0
2	C	416	TYR	2.0

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

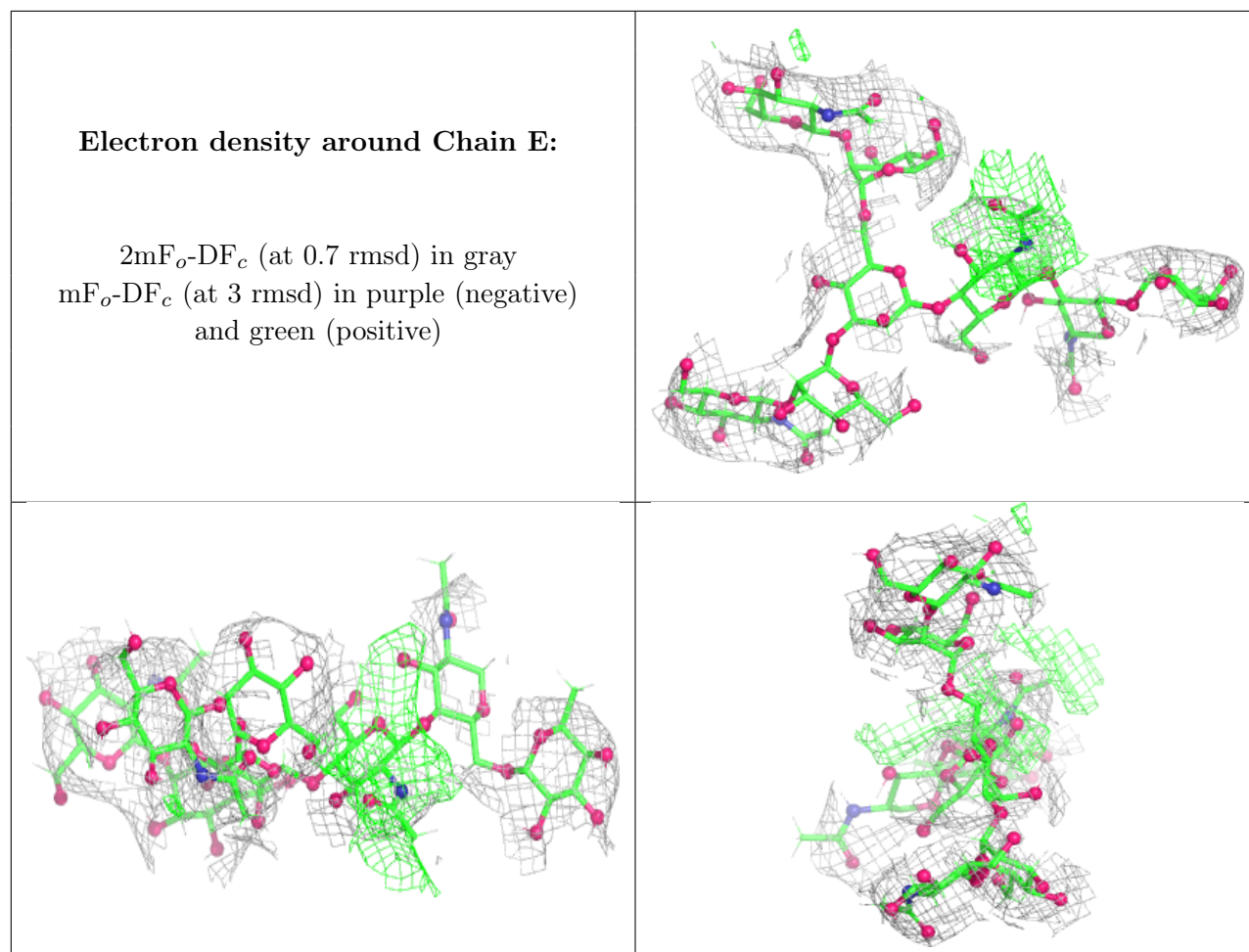
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	NAG	E	1	14/15	0.78	0.10	30,158,163,163	1
3	NAG	E	2	14/15	0.82	0.19	30,168,173,174	2
3	NAG	E	7	14/15	0.82	0.12	30,164,171,173	3
3	NAG	E	5	14/15	0.88	0.09	30,159,163,166	3
3	MAN	E	6	11/12	0.91	0.10	30,159,161,167	3
3	MAN	E	4	11/12	0.92	0.08	30,143,148,154	3
3	BMA	E	3	11/12	0.92	0.07	30,151,155,156	2
3	FUC	E	8	10/11	0.94	0.10	30,133,136,136	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.