



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:19 AM BST

PDB ID : 6W3H
Title : Brain delivery of therapeutic proteins using an Fc fragment blood-brain barrier transport vehicle in mice and monkeys
Authors : Srivastava, A.; Kariolis, M.; Wells, R.
Deposited on : 2020-03-09
Resolution : 3.38 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

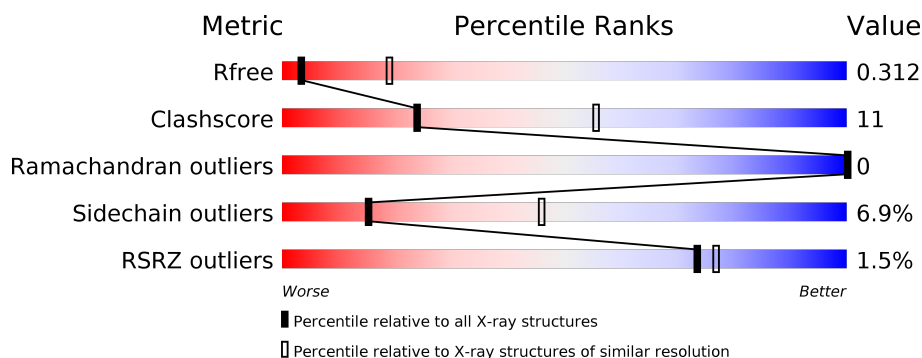
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 on 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	<div> <div>65%</div> <div>25%</div> <div>8%</div> </div>
1	B	227	<div>4%</div> <div>66%</div> <div>17%</div> <div>16%</div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5251 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 ATV Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1623	1040	263	315	5			
1	B	190	Total	C	N	O	S	0	0	0
			1464	941	237	281	5			

- Molecule 2 is a protein called Transferrin receptor protein 1,Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	144	Total	C	N	O	S	0	0	0
			1006	627	173	202	4			
2	D	147	Total	C	N	O	S	0	0	0
			1069	678	184	202	5			

There are 18 discrepancies between the modelled and reference sequences:

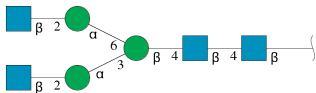
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	THR	-	expression tag	UNP P02786
C	179	ALA	-	linker	UNP P02786
C	180	SER	-	linker	UNP P02786
C	181	HIS	-	expression tag	UNP P02786
C	182	HIS	-	expression tag	UNP P02786
C	183	HIS	-	expression tag	UNP P02786
C	184	HIS	-	expression tag	UNP P02786
C	185	HIS	-	expression tag	UNP P02786
C	186	HIS	-	expression tag	UNP P02786
D	21	THR	-	expression tag	UNP P02786
D	179	ALA	-	linker	UNP P02786
D	180	SER	-	linker	UNP P02786
D	181	HIS	-	expression tag	UNP P02786
D	182	HIS	-	expression tag	UNP P02786
D	183	HIS	-	expression tag	UNP P02786
D	184	HIS	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
D	185	HIS	-	expression tag	UNP P02786
D	186	HIS	-	expression tag	UNP P02786

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.

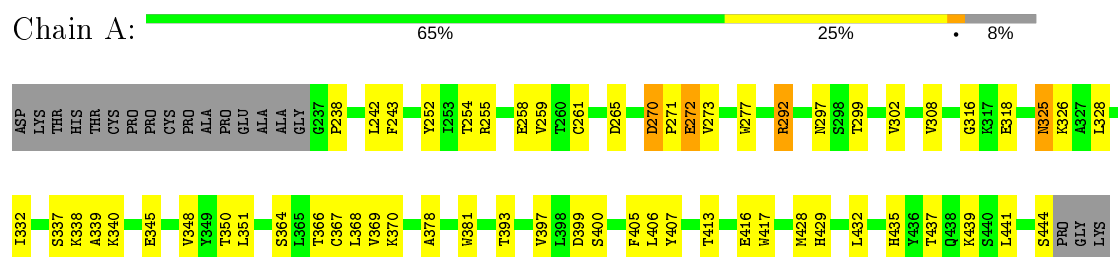


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	0	0	0
			89	50	4	35			

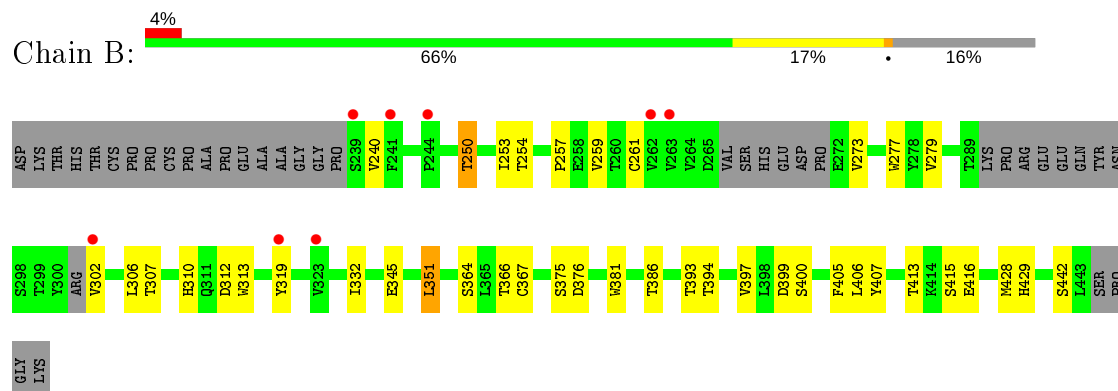
3 Residue-property plots

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.

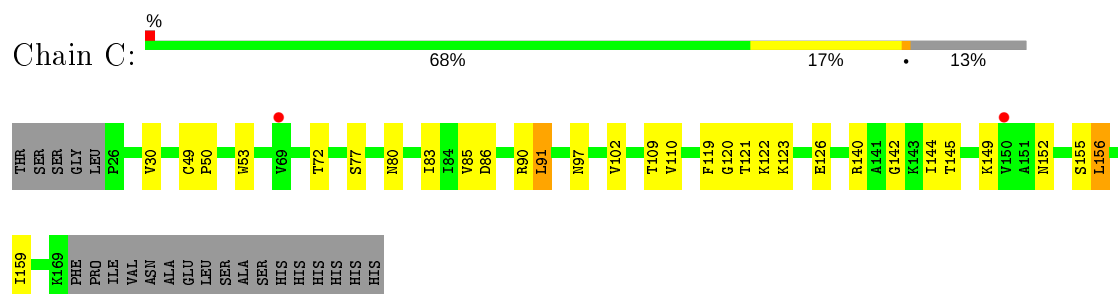
- Molecule 1: ATV Fc



- Molecule 1: ATV Fc

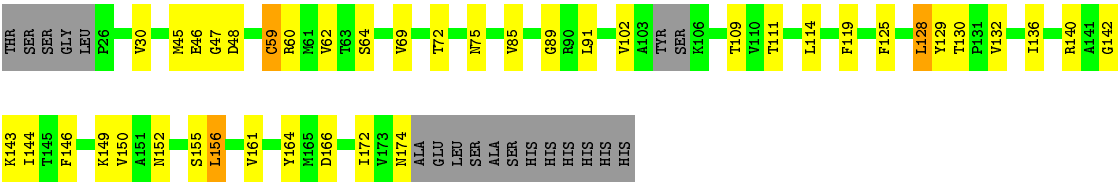


- Molecule 2: Transferrin receptor protein 1,Transferrin receptor protein 1

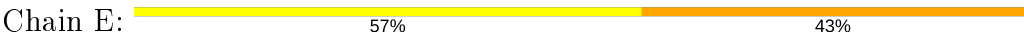


- Molecule 2: Transferrin receptor protein 1,Transferrin receptor protein 1





● 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)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	126.37Å 126.37Å 113.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.30 – 3.38 55.24 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.30-3.38) 99.8 (55.24-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.238 , 0.318 0.236 , 0.312	Depositor DCC
R_{free} test set	657 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	87.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5251	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.66	0/1670	0.81	0/2284
1	B	0.66	0/1504	0.79	0/2057
2	C	0.67	0/1020	0.87	0/1396
2	D	0.67	0/1085	0.94	0/1477
All	All	0.67	0/5279	0.84	0/7214

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	1623	0	1534	41	0
1	B	1464	0	1363	24	0
2	C	1006	0	923	28	0
2	D	1069	0	1057	25	0
3	E	89	0	76	3	0
All	All	5251	0	4953	113	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 11.

All (113) 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)
1:B:273:VAL:HG21	1:B:302:VAL:HG11	1.70	0.73
2:C:119:PHE:HD2	2:C:142:GLY:HA3	1.54	0.72
2:D:30:VAL:HG21	2:D:150:VAL:HG21	1.75	0.69
1:B:240:VAL:HG21	1:B:332:ILE:HD11	1.75	0.67
2:C:72:THR:HG23	2:C:109:THR:HG22	1.74	0.67
3:E:2:NAG:H82	3:E:6:MAN:O4	1.94	0.67
2:C:119:PHE:CD2	2:C:142:GLY:HA3	2.29	0.66
2:D:30:VAL:HG22	2:D:161:VAL:HB	1.77	0.65
2:D:59:CYS:SG	2:D:59:CYS:O	2.55	0.64
2:D:30:VAL:HG21	2:D:150:VAL:CG2	2.27	0.64
1:A:413:THR:HG23	1:A:416:GLU:HG3	1.81	0.63
1:A:351:LEU:N	1:A:351:LEU:HD12	2.14	0.63
1:A:238:PRO:HA	1:A:265:ASP:O	2.01	0.60
2:D:69:VAL:HG13	2:D:136:ILE:HD12	1.84	0.60
1:A:328:LEU:HD21	1:A:332:ILE:HD12	1.84	0.60
1:A:413:THR:CG2	1:A:416:GLU:HG3	2.32	0.60
2:D:45:MET:HE3	2:D:114:LEU:HB3	1.84	0.59
2:C:30:VAL:HG13	2:C:102:VAL:HG11	1.84	0.59
2:C:83:ILE:HD12	2:C:91:LEU:HD13	1.85	0.58
1:A:366:THR:HG23	1:B:407:TYR:CZ	2.39	0.58
2:C:121:THR:HG22	2:C:123:LYS:H	1.68	0.58
1:A:350:THR:C	1:A:351:LEU:HD12	2.25	0.57
1:A:318:GLU:HA	1:A:337:SER:HB3	1.86	0.57
1:A:252:TYR:HB2	1:A:255:ARG:HG3	1.87	0.55
1:A:397:VAL:HB	1:A:405:PHE:CE1	2.41	0.55
2:D:125:PHE:HE1	2:D:132:VAL:HG21	1.71	0.55
1:A:316:GLY:O	1:A:340:LYS:HE3	2.08	0.54
1:A:368:LEU:HD23	1:A:368:LEU:C	2.29	0.53
2:C:91:LEU:HD22	1:B:386:THR:HB	1.90	0.53
1:B:257:PRO:HD3	1:B:310:HIS:NE2	2.23	0.52
2:D:152:ASN:O	2:D:156:LEU:HD12	2.09	0.52
1:A:345:GLU:HG3	1:A:432:LEU:HD23	1.91	0.52
2:C:122:LYS:H	2:C:122:LYS:HD2	1.73	0.52
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.45	0.52
1:A:297:ASN:OD1	1:A:299:THR:OG1	2.17	0.52
2:C:120:GLY:O	2:C:152:ASN:ND2	2.36	0.51
2:C:53:TRP:N	2:C:53:TRP:CD1	2.77	0.51
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.45	0.51
1:B:253:ILE:HA	1:B:310:HIS:CE1	2.46	0.51
2:D:140:ARG:HD3	2:D:166:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:O	1:A:325:ASN:ND2	2.44	0.51
2:D:85:VAL:CG1	2:D:89:GLY:HA2	2.41	0.50
2:C:126:GLU:HA	2:C:126:GLU:OE1	2.10	0.50
1:B:397:VAL:HB	1:B:405:PHE:CE1	2.45	0.50
1:A:242:LEU:HD11	1:A:259:VAL:CG1	2.42	0.50
1:A:243:PHE:HD2	3:E:7:NAG:H62	1.76	0.50
1:B:413:THR:OG1	1:B:416:GLU:HG3	2.11	0.50
2:D:47:GLY:O	2:D:60:ARG:CD	2.60	0.50
1:B:351:LEU:HD12	1:B:366:THR:HB	1.93	0.49
2:C:144:ILE:HG22	2:C:145:THR:O	2.11	0.49
1:A:243:PHE:CD2	3:E:7:NAG:H62	2.46	0.49
2:D:174:ASN:N	2:D:174:ASN:OD1	2.45	0.49
2:C:85:VAL:HA	2:C:90:ARG:O	2.13	0.49
1:A:270:ASP:OD2	1:A:326:LYS:CB	2.61	0.48
1:B:279:VAL:HG22	1:B:319:TYR:CD1	2.48	0.48
2:D:140:ARG:HG2	2:D:164:TYR:CZ	2.48	0.48
2:D:125:PHE:CE1	2:D:132:VAL:HG21	2.49	0.48
2:D:62:VAL:HG11	2:D:130:THR:HG21	1.95	0.48
2:C:30:VAL:HG22	2:C:102:VAL:HG21	1.95	0.48
2:C:122:LYS:H	2:C:122:LYS:CD	2.26	0.47
2:C:152:ASN:O	2:C:156:LEU:HD12	2.14	0.47
2:C:80:ASN:O	2:C:97:ASN:ND2	2.47	0.47
2:C:121:THR:HA	2:C:144:ILE:HD11	1.97	0.47
2:C:30:VAL:CG1	2:C:102:VAL:HG11	2.46	0.46
2:C:119:PHE:CE2	2:C:140:ARG:HG3	2.50	0.46
2:C:122:LYS:HD2	2:C:122:LYS:N	2.30	0.46
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.51	0.46
1:A:366:THR:HG21	1:B:407:TYR:CE1	2.50	0.46
1:A:417:TRP:HH2	1:A:441:LEU:HD11	1.81	0.46
1:A:271:PRO:HB2	1:A:292:ARG:NH1	2.31	0.46
1:A:297:ASN:O	1:A:299:THR:HG23	2.15	0.46
2:C:144:ILE:O	2:C:149:LYS:HE2	2.16	0.46
1:B:393:THR:HG23	1:B:406:LEU:HD13	1.98	0.45
2:D:30:VAL:HG12	2:D:102:VAL:HG21	1.98	0.45
2:D:47:GLY:O	2:D:60:ARG:HD2	2.17	0.45
2:D:47:GLY:O	2:D:60:ARG:HD3	2.17	0.45
1:B:406:LEU:HD12	1:B:406:LEU:C	2.36	0.45
2:D:128:LEU:HD12	2:D:129:TYR:N	2.31	0.44
1:A:429:HIS:O	1:A:435:HIS:HA	2.17	0.44
1:A:252:TYR:CB	1:A:255:ARG:HG3	2.48	0.44
1:B:259:VAL:HG23	1:B:306:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:110:VAL:HG11	2:C:159:ILE:HG13	2.00	0.44
1:A:393:THR:HG23	1:A:406:LEU:HD13	2.01	0.43
2:C:86:ASP:HB3	2:C:90:ARG:H	1.82	0.43
1:A:273:VAL:HG21	1:A:302:VAL:HG11	1.99	0.43
2:D:119:PHE:CD1	2:D:142:GLY:HA3	2.53	0.43
2:D:140:ARG:CD	2:D:166:ASP:OD2	2.67	0.43
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.53	0.43
1:B:376:ASP:O	1:B:429:HIS:HD2	2.02	0.43
2:C:119:PHE:CE1	2:C:140:ARG:HD3	2.54	0.43
2:C:49:CYS:HA	2:C:50:PRO:HD3	1.87	0.43
1:B:279:VAL:HG22	1:B:319:TYR:CE1	2.54	0.43
1:B:351:LEU:HD12	1:B:366:THR:CG2	2.49	0.42
2:D:72:THR:OG1	2:D:109:THR:HG23	2.18	0.42
1:A:338:LYS:NZ	1:A:339:ALA:O	2.47	0.42
1:B:406:LEU:HD12	1:B:407:TYR:N	2.34	0.42
1:A:368:LEU:HD21	1:A:370:LYS:HB3	2.00	0.42
1:A:259:VAL:HG23	1:A:308:VAL:HG11	2.00	0.42
1:A:406:LEU:HD12	1:A:406:LEU:C	2.39	0.42
1:B:250:THR:HG21	1:B:313:TRP:CD1	2.55	0.42
1:A:397:VAL:HG21	1:B:394:THR:HA	2.02	0.42
1:A:348:VAL:O	1:A:439:LYS:HG3	2.20	0.41
2:D:143:LYS:O	2:D:172:ILE:HA	2.20	0.41
1:A:368:LEU:HD23	1:A:369:VAL:N	2.34	0.41
2:C:86:ASP:HB2	2:C:90:ARG:HB2	2.02	0.41
1:A:366:THR:HG23	1:B:407:TYR:OH	2.20	0.41
2:D:144:ILE:O	2:D:149:LYS:HE2	2.20	0.41
2:D:146:PHE:O	2:D:150:VAL:HG23	2.21	0.40
1:A:366:THR:CG2	1:B:407:TYR:CE1	3.04	0.40
1:A:406:LEU:HD12	1:A:407:TYR:N	2.36	0.40
1:A:351:LEU:N	1:A:351:LEU:CD1	2.81	0.40
1:A:378:ALA:HB3	1:A:428:MET:HB2	2.02	0.40
2:C:90:ARG:HG3	2:C:90:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/227 (91%)	205 (100%)	1 (0%)	0	100	100
1	B	182/227 (80%)	180 (99%)	2 (1%)	0	100	100
2	C	142/166 (86%)	136 (96%)	6 (4%)	0	100	100
2	D	143/166 (86%)	139 (97%)	4 (3%)	0	100	100
All	All	673/786 (86%)	660 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/207 (87%)	170 (94%)	11 (6%)	18	49
1	B	160/207 (77%)	147 (92%)	13 (8%)	11	38
2	C	98/140 (70%)	94 (96%)	4 (4%)	30	61
2	D	112/140 (80%)	102 (91%)	10 (9%)	9	34
All	All	551/694 (79%)	513 (93%)	38 (7%)	15	46

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	THR
1	A	258	GLU
1	A	270	ASP
1	A	272	GLU
1	A	292	ARG
1	A	325	ASN
1	A	364	SER
1	A	399	ASP

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Mol	Chain	Res	Type
1	A	400	SER
1	A	437	THR
1	A	444	SER
2	C	77	SER
2	C	91	LEU
2	C	155	SER
2	C	156	LEU
2	D	46	GLU
2	D	48	ASP
2	D	59	CYS
2	D	64	SER
2	D	75	ASN
2	D	91	LEU
2	D	111	THR
2	D	128	LEU
2	D	155	SER
2	D	156	LEU
1	B	250	THR
1	B	254	THR
1	B	307	THR
1	B	312	ASP
1	B	345	GLU
1	B	351	LEU
1	B	364	SER
1	B	375	SER
1	B	399	ASP
1	B	400	SER
1	B	415	SER
1	B	428	MET
1	B	442	SER

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

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 ⓘ

7 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	0.88	1 (7%)	17,19,21	1.85	5 (29%)
3	NAG	E	2	3	14,14,15	0.73	0	17,19,21	1.25	3 (17%)
3	BMA	E	3	3	11,11,12	0.84	1 (9%)	15,15,17	1.96	6 (40%)
3	MAN	E	4	3	11,11,12	0.57	0	15,15,17	1.96	5 (33%)
3	NAG	E	5	3	14,14,15	0.74	0	17,19,21	1.84	6 (35%)
3	MAN	E	6	3	11,11,12	0.65	0	15,15,17	1.81	4 (26%)
3	NAG	E	7	3	14,14,15	0.45	0	17,19,21	1.93	6 (35%)

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	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	1/6/23/26	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	NAG	E	7	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C2-C3	2.19	1.55	1.52
3	E	1	NAG	C4-C5	2.16	1.57	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	NAG	C1-C2-N2	-4.78	102.33	110.49
3	E	4	MAN	O2-C2-C3	-4.43	101.26	110.14
3	E	1	NAG	C4-C3-C2	-3.78	105.47	111.02
3	E	3	BMA	C6-C5-C4	-3.52	104.77	113.00
3	E	6	MAN	C2-C3-C4	-3.47	104.88	110.89
3	E	5	NAG	C1-C2-N2	3.47	116.42	110.49
3	E	3	BMA	O3-C3-C2	3.43	116.57	109.99
3	E	6	MAN	O3-C3-C2	-3.15	103.97	109.99
3	E	6	MAN	O3-C3-C4	3.11	117.54	110.35
3	E	4	MAN	O3-C3-C2	-3.01	104.23	109.99
3	E	5	NAG	C4-C3-C2	2.97	115.38	111.02
3	E	4	MAN	C1-C2-C3	2.94	113.28	109.67
3	E	3	BMA	C2-C3-C4	-2.85	105.97	110.89
3	E	7	NAG	O5-C1-C2	-2.84	106.80	111.29
3	E	5	NAG	C3-C4-C5	2.83	115.29	110.24
3	E	5	NAG	O5-C5-C6	2.82	111.63	107.20
3	E	1	NAG	O6-C6-C5	2.81	120.94	111.29
3	E	1	NAG	C1-O5-C5	2.67	115.81	112.19
3	E	7	NAG	C6-C5-C4	-2.66	106.77	113.00
3	E	3	BMA	O5-C5-C6	2.62	111.31	107.20
3	E	5	NAG	O3-C3-C2	-2.57	104.15	109.47
3	E	7	NAG	O7-C7-N2	2.57	126.67	121.95
3	E	4	MAN	O5-C1-C2	-2.53	106.87	110.77
3	E	1	NAG	O4-C4-C5	2.49	115.49	109.30
3	E	2	NAG	C3-C4-C5	-2.49	105.80	110.24
3	E	1	NAG	O5-C1-C2	-2.47	107.38	111.29
3	E	6	MAN	O5-C1-C2	-2.46	106.97	110.77
3	E	5	NAG	C1-O5-C5	-2.45	108.87	112.19
3	E	7	NAG	C4-C3-C2	-2.44	107.44	111.02
3	E	2	NAG	O3-C3-C4	2.43	115.96	110.35
3	E	3	BMA	O3-C3-C4	-2.41	104.78	110.35
3	E	4	MAN	C3-C4-C5	2.33	114.39	110.24
3	E	2	NAG	O5-C1-C2	-2.32	107.62	111.29
3	E	3	BMA	O5-C1-C2	-2.12	107.49	110.77
3	E	7	NAG	O7-C7-C8	-2.01	118.32	122.06

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	7	NAG	O5-C5-C6-O6
3	E	7	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

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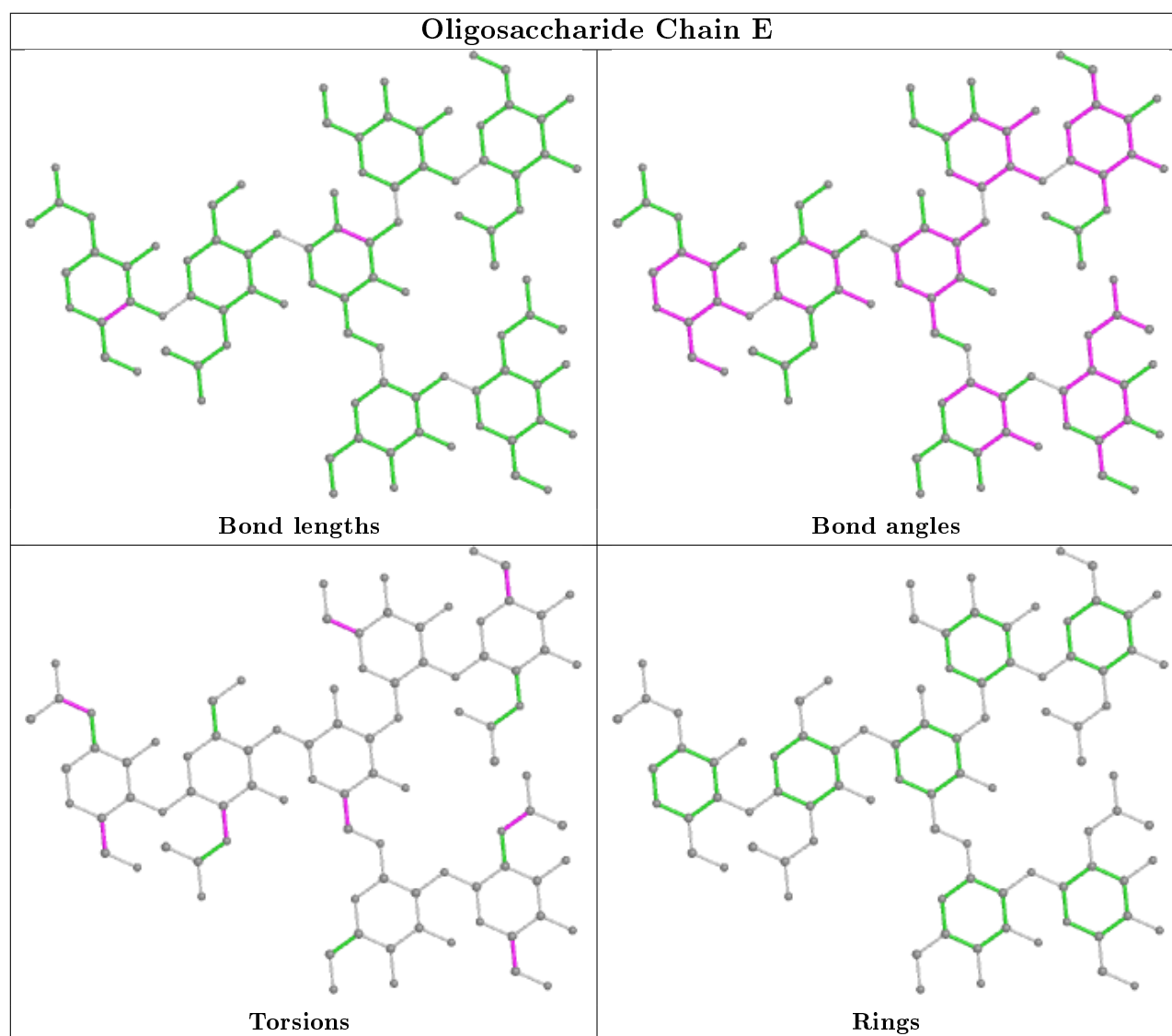
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	E	7	NAG	C8-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0
3	E	7	NAG	2	0
3	E	6	MAN	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](#)

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 [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	A	208/227 (91%)	0.09	0 100 100	57, 71, 112, 132	1 (0%)
1	B	190/227 (83%)	0.29	8 (4%) 36 40	51, 74, 129, 139	0
2	C	144/166 (86%)	0.30	2 (1%) 75 79	62, 89, 125, 143	0
2	D	147/166 (88%)	0.08	0 100 100	55, 73, 111, 133	0
All	All	689/786 (87%)	0.19	10 (1%) 73 77	51, 76, 124, 143	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	3.5
1	B	239	SER	3.5
1	B	262	VAL	3.4
1	B	302	VAL	2.9
1	B	323	VAL	2.5
1	B	319	TYR	2.3
2	C	150	VAL	2.3
1	B	241	PHE	2.2
1	B	244	PRO	2.1
2	C	69	VAL	2.1

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

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

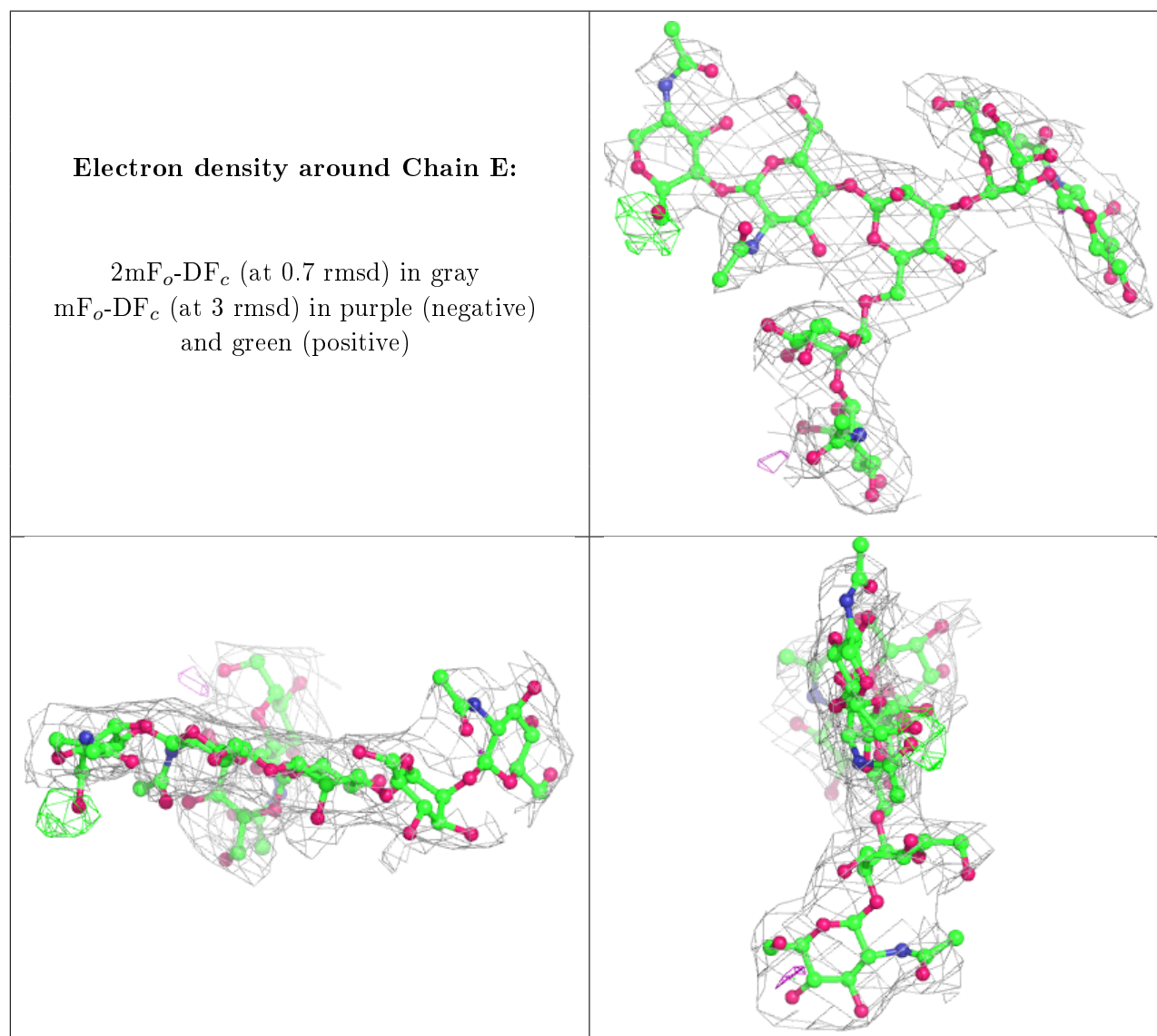
6.3 Carbohydrates [i](#)

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	0.71	0.23	82,92,97,99	0
3	NAG	E	5	14/15	0.83	0.22	91,98,100,102	0
3	NAG	E	2	14/15	0.89	0.23	79,86,91,95	0
3	MAN	E	4	11/12	0.90	0.14	84,86,90,95	0
3	NAG	E	7	14/15	0.90	0.20	71,78,93,95	0
3	MAN	E	6	11/12	0.92	0.17	80,84,88,89	0
3	BMA	E	3	11/12	0.93	0.15	77,78,81,82	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.