



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:20 PM UTC

PDB ID : 6W3H / pdb_00006w3h
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 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

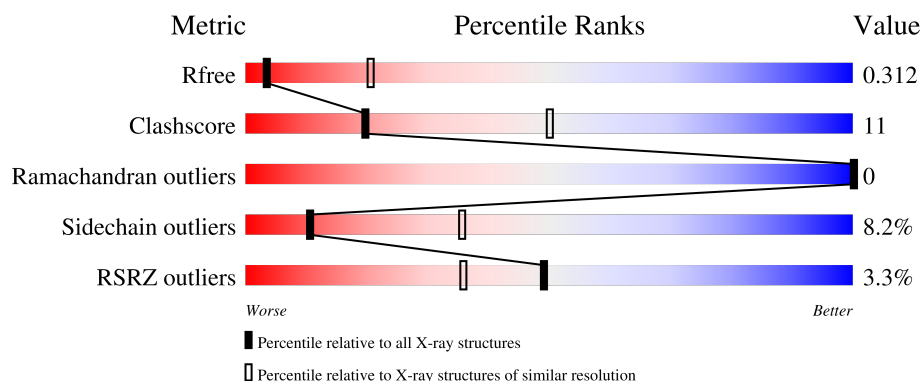
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	% 63% 26% • 8%
1	B	227	4% 63% 18% • 16%
2	C	166	5% 66% 17% • • 13%
2	D	166	% 60% 27% • 11%
3	E	7	57% 43%

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:

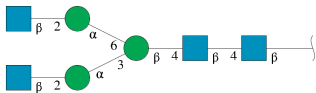
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	THR	-	expression tag	UNP P02786
C	179	ALA	-	linker	UNP P02786
C	180	SER	-	linker	UNP P02786
C	181	HIS	-	expression tag	UNP P02786
C	182	HIS	-	expression tag	UNP P02786
C	183	HIS	-	expression tag	UNP P02786
C	184	HIS	-	expression tag	UNP P02786
C	185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

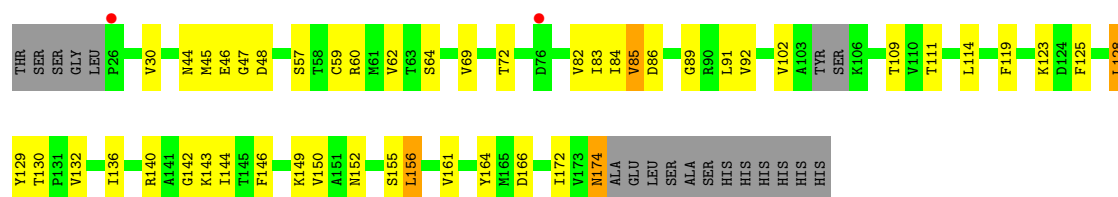
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

Chain D: 



- 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

Chain E: 



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 55.30 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (55.30-3.38) 99.8 (55.30-3.38)	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 (4.52%)	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 , 60.1	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: NAG, MAN, BMA

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	0.98	1/1670 (0.1%)	1.22	5/2284 (0.2%)
1	B	0.96	0/1504	1.16	3/2057 (0.1%)
2	C	1.00	0/1020	1.38	6/1396 (0.4%)
2	D	1.00	3/1085 (0.3%)	1.45	4/1477 (0.3%)
All	All	0.98	4/5279 (0.1%)	1.28	18/7214 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	PRO	C-O	-6.63	1.17	1.23
2	D	83	ILE	C-O	-5.90	1.18	1.23
2	D	57	SER	C-O	5.09	1.30	1.24
2	D	123	LYS	C-O	5.05	1.29	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	85	VAL	CA-C-N	7.17	132.19	120.94
2	C	85	VAL	C-N-CA	7.17	132.19	120.94
2	D	86	ASP	CA-CB-CG	6.95	119.55	112.60
2	D	85	VAL	CA-C-N	6.34	130.90	120.94
2	D	85	VAL	C-N-CA	6.34	130.90	120.94
2	C	97	ASN	CB-CA-C	6.30	117.20	110.65
2	C	86	ASP	CA-CB-CG	6.27	118.87	112.60
2	D	92	VAL	N-CA-C	-5.88	106.97	111.62
1	B	241	PHE	CA-CB-CG	5.79	119.59	113.80
1	B	401	ASP	CA-CB-CG	5.55	118.16	112.60
1	A	355	ARG	N-CA-C	-5.51	105.37	111.71
2	C	62	VAL	CA-C-O	-5.40	116.28	121.63
1	B	359	THR	CA-CB-OG1	-5.37	101.54	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ASP	CA-CB-CG	5.30	117.90	112.60
2	C	50	PRO	CB-CA-C	-5.24	104.11	110.98
1	A	292	ARG	CA-C-N	-5.21	114.68	122.39
1	A	292	ARG	C-N-CA	-5.21	114.68	122.39
1	A	318	GLU	CB-CA-C	-5.10	101.44	109.80

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	25	0
2	C	1006	0	923	29	0
2	D	1069	0	1057	27	0
3	E	89	0	76	3	0
All	All	5251	0	4953	117	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 (117) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:THR:HG23	1:A:416:GLU:HG3	1.81	0.63
1:A:351:LEU:HD12	1:A:351:LEU:N	2.14	0.63
2:D:45:MET:HE3	2:D:114:LEU:HB3	1.80	0.63
1:A:350:THR:C	1:A:351:LEU:HD12	2.25	0.62
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: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:368:LEU:C	1:A:368:LEU:HD23	2.29	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
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:HD2	2:C:122:LYS:H	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:CD1	2:C:53:TRP:N	2.77	0.51
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.45	0.51
2:D:140:ARG:HD3	2:D:166:ASP:OD2	2.11	0.51
1:B:253:ILE:HA	1:B:310:HIS:CE1	2.46	0.51
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:B:406:LEU:HD12	1:B:406:LEU:C	2.36	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
2:C:144:ILE:HG22	2:C:145:THR:O	2.11	0.49
1:B:351:LEU:HD12	1:B:366:THR:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:140:ARG:HG2	2:D:164:TYR:CZ	2.48	0.48
1:B:279:VAL:HG22	1:B:319:TYR:CD1	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
1:A:406:LEU:C	1:A:406:LEU:HD12	2.39	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
1:B:252:TYR:OH	1:B:428:MET:HE2	2.16	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
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
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:C:56:ASP:C	2:C:58:THR:H	2.26	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
2:C:49:CYS:HA	2:C:50:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:PHE:CE1	2:C:140:ARG:HD3	2.54	0.43
1:B:376:ASP:O	1:B:429:HIS:HD2	2.02	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
2:D:44:ASN:CG	2:D:84:ILE:HD13	2.45	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
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
1:A:368:LEU:HD23	1:A:369:VAL:N	2.34	0.41
2:D:85:VAL:HG13	2:D:89:GLY:C	2.46	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:HH11	2:C:90:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/227 (91%)	205 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	168 (93%)	13 (7%)	13	39
1	B	160/207 (77%)	144 (90%)	16 (10%)	7	26
2	C	98/140 (70%)	92 (94%)	6 (6%)	17	43
2	D	112/140 (80%)	102 (91%)	10 (9%)	9	31
All	All	551/694 (79%)	506 (92%)	45 (8%)	10	36

All (45) 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	308	VAL
1	A	317	LYS
1	A	335	THR
1	A	364	SER
1	A	400	SER
1	A	437	THR
1	A	441	LEU
1	A	444	SER

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Mol	Chain	Res	Type
2	C	77	SER
2	C	82	VAL
2	C	85	VAL
2	C	91	LEU
2	C	155	SER
2	C	156	LEU
2	D	46	GLU
2	D	48	ASP
2	D	64	SER
2	D	82	VAL
2	D	91	LEU
2	D	111	THR
2	D	128	LEU
2	D	155	SER
2	D	156	LEU
2	D	174	ASN
1	B	250	THR
1	B	254	THR
1	B	263	VAL
1	B	307	THR
1	B	308	VAL
1	B	312	ASP
1	B	332	ILE
1	B	345	GLU
1	B	351	LEU
1	B	364	SER
1	B	375	SER
1	B	409	LYS
1	B	413	THR
1	B	415	SER
1	B	428	MET
1	B	442	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	286	ASN
2	D	68	ASN
2	D	133	ASN
1	B	419	GLN

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	1.86	6 (35%)
3	NAG	E	2	3	14,14,15	0.74	0	17,19,21	1.24	3 (17%)
3	BMA	E	3	3	11,11,12	0.82	1 (9%)	15,15,17	1.79	4 (26%)
3	MAN	E	4	3	11,11,12	0.56	0	15,15,17	1.80	4 (26%)
3	NAG	E	5	3	14,14,15	0.77	1 (7%)	17,19,21	1.81	6 (35%)
3	MAN	E	6	3	11,11,12	0.63	0	15,15,17	1.70	3 (20%)
3	NAG	E	7	3	14,14,15	0.46	0	17,19,21	2.00	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	-	2/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	7	3	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	C4-C5	2.14	1.57	1.53
3	E	3	BMA	C2-C3	2.13	1.55	1.52
3	E	5	NAG	C1-C2	2.04	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7	NAG	C1-C2-N2	-5.14	102.33	110.43
3	E	4	MAN	O2-C2-C3	-4.29	101.26	110.15
3	E	5	NAG	C1-C2-N2	3.80	116.42	110.43
3	E	1	NAG	C4-C3-C2	-3.78	105.47	111.02
3	E	6	MAN	C2-C3-C4	-3.40	104.88	110.86
3	E	3	BMA	C6-C5-C4	-3.36	104.77	113.02
3	E	3	BMA	O3-C3-C2	3.19	116.57	110.05
3	E	6	MAN	O3-C3-C4	3.04	117.54	110.38
3	E	6	MAN	O3-C3-C2	-2.98	103.97	110.05
3	E	5	NAG	C4-C3-C2	2.97	115.38	111.02
3	E	7	NAG	O5-C1-C2	-2.90	106.80	111.29
3	E	4	MAN	O3-C3-C2	-2.85	104.23	110.05
3	E	1	NAG	O6-C6-C5	2.82	120.94	111.33
3	E	5	NAG	C3-C4-C5	2.79	115.29	110.23
3	E	3	BMA	C2-C3-C4	-2.78	105.97	110.86
3	E	1	NAG	C1-O5-C5	2.70	115.81	112.19
3	E	7	NAG	O7-C7-N2	2.66	126.67	121.98
3	E	7	NAG	C6-C5-C4	-2.55	106.77	113.02
3	E	5	NAG	O3-C3-C2	-2.53	104.15	109.40
3	E	1	NAG	O5-C1-C2	-2.53	107.38	111.29
3	E	1	NAG	O4-C4-C5	2.50	115.49	109.32
3	E	4	MAN	C1-C2-C3	2.50	113.28	109.64
3	E	5	NAG	C1-O5-C5	-2.47	108.87	112.19
3	E	2	NAG	C3-C4-C5	-2.44	105.80	110.23
3	E	7	NAG	C4-C3-C2	-2.44	107.44	111.02
3	E	3	BMA	O3-C3-C4	-2.37	104.78	110.38
3	E	2	NAG	O5-C1-C2	-2.37	107.62	111.29
3	E	2	NAG	O3-C3-C4	2.37	115.96	110.38
3	E	4	MAN	C3-C4-C5	2.29	114.39	110.23
3	E	7	NAG	O7-C7-C8	-2.10	118.32	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	NAG	O5-C5-C6	2.04	111.63	107.66
3	E	1	NAG	O3-C3-C2	2.02	113.59	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

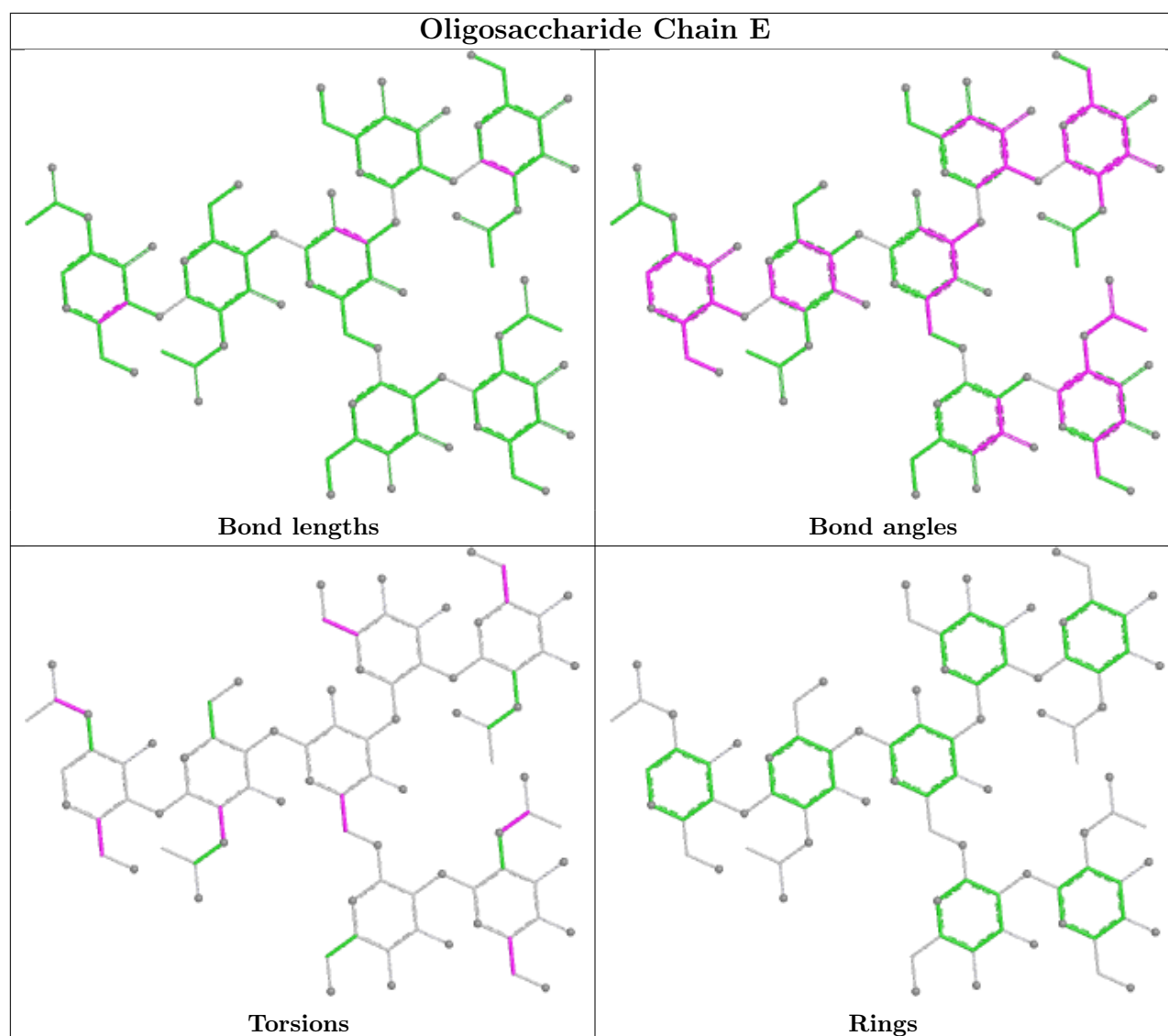
Mol	Chain	Res	Type	Atoms
3	E	7	NAG	O5-C5-C6-O6
3	E	7	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	E	7	NAG	C8-C7-N2-C2
3	E	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	NAG	2	0
3	E	2	NAG	1	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 ⓘ

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	208/227 (91%)	0.37	3 (1%) 73 59	57, 71, 112, 132	1 (0%)
1	B	190/227 (83%)	0.61	9 (4%) 36 27	51, 74, 129, 139	0
2	C	144/166 (86%)	0.56	9 (6%) 26 20	62, 89, 125, 143	0
2	D	147/166 (88%)	0.44	2 (1%) 73 59	55, 73, 111, 133	0
All	All	689/786 (87%)	0.49	23 (3%) 49 36	51, 76, 124, 143	1 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	3.8
2	C	56	ASP	3.3
1	B	242	LEU	3.1
2	C	166	ASP	3.1
1	B	244	PRO	2.9
1	B	262	VAL	2.8
1	B	300	TYR	2.8
1	B	281	GLY	2.6
2	C	165	MET	2.5
1	B	302	VAL	2.4
2	D	76	ASP	2.4
1	A	399	ASP	2.4
2	C	104	TYR	2.3
2	C	26	PRO	2.3
2	C	58	THR	2.2
1	B	241	PHE	2.1
1	A	264	VAL	2.1
1	B	283	GLU	2.1
1	B	240	VAL	2.1
2	C	129	TYR	2.1
2	C	168	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	26	PRO	2.1
2	C	155	SER	2.0

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

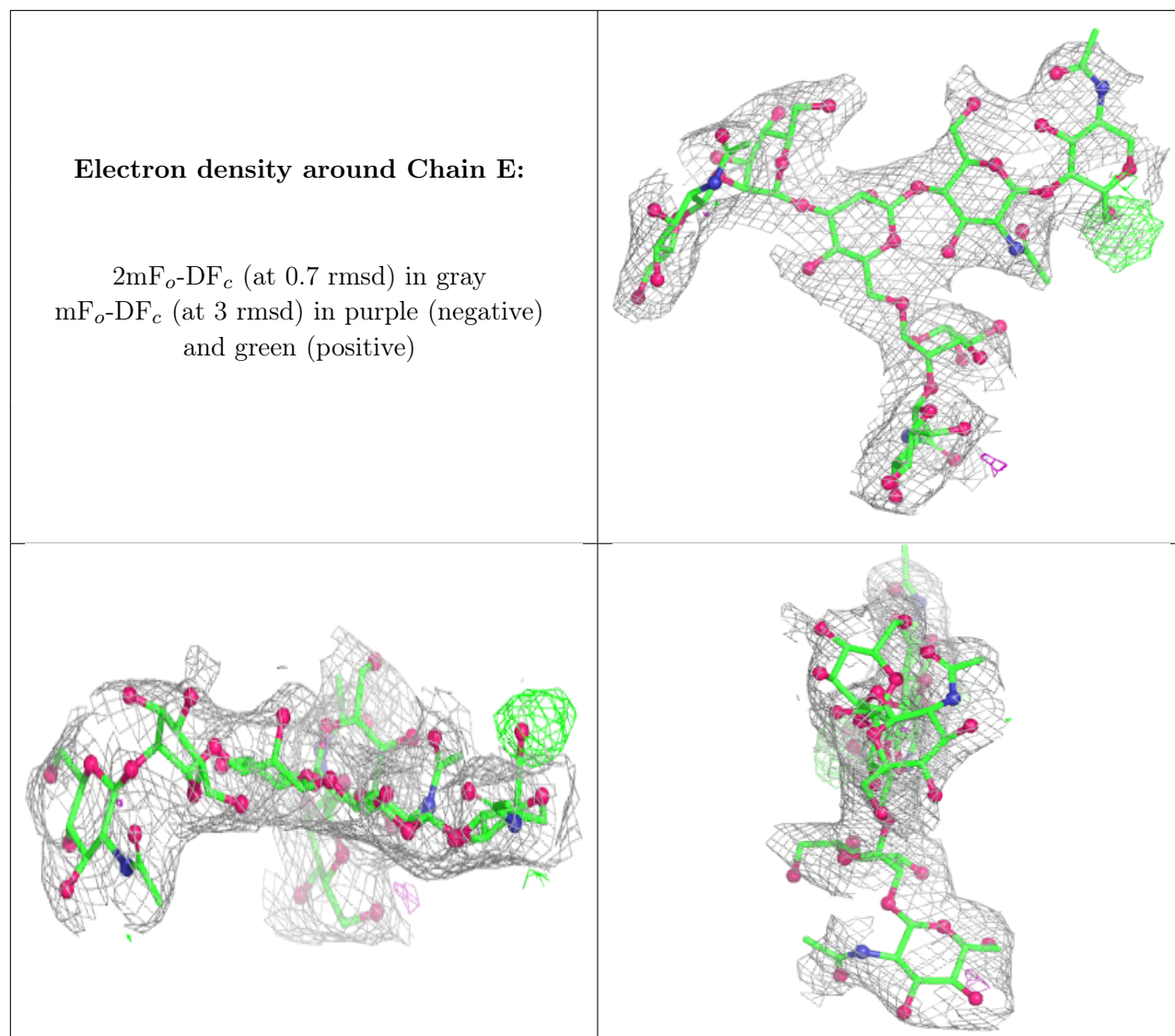
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
3	NAG	E	5	14/15	0.60	0.14	91,98,100,102	0
3	NAG	E	1	14/15	0.73	0.14	82,92,97,99	0
3	NAG	E	7	14/15	0.84	0.13	71,78,93,95	0
3	MAN	E	4	11/12	0.86	0.08	84,86,90,95	0
3	MAN	E	6	11/12	0.87	0.10	80,84,88,89	0
3	NAG	E	2	14/15	0.88	0.10	79,86,91,95	0
3	BMA	E	3	11/12	0.94	0.08	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.