



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:18 PM UTC

PDB ID : 3ZP6 / pdb_00003zp6
Title : INFLUENZA VIRUS (VN1194) H5 E190D mutant HA with LSTc
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Deposited on : 2013-02-26
Resolution : 2.60 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

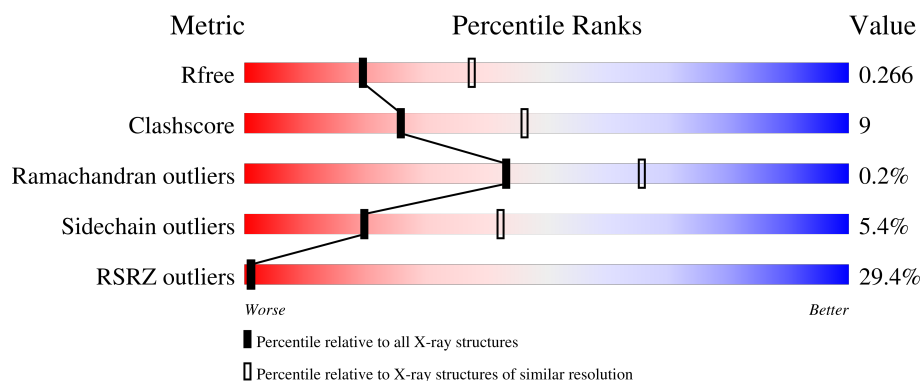
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	E	340	34% 75% 17% 6%
2	F	160	17% 82% 14% ..
3	A	2	50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4007 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 HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	321	Total	C	N	O	S	0	0	0
			2548	1610	440	483	15			

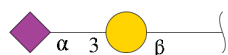
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	LYS	THR	conflict	UNP Q6DQ34
E	190	ASP	GLU	engineered mutation	UNP Q6DQ34

- Molecule 2 is a protein called HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	158	Total	C	N	O	S	0	0	0
			1272	791	221	252	8			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

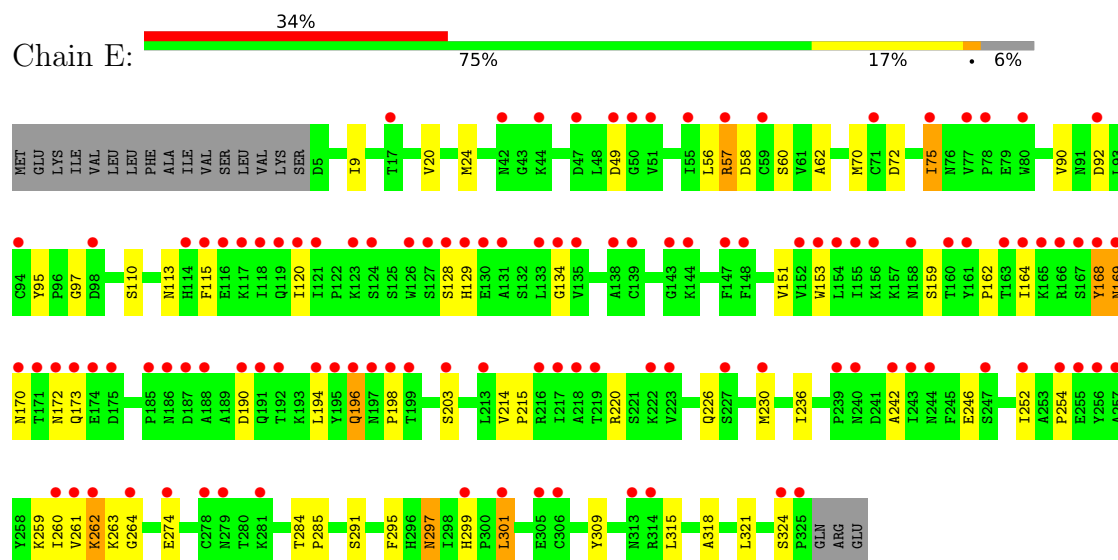
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	72	Total	O	0	0
			72	72		
5	F	62	Total	O	0	0
			62	62		

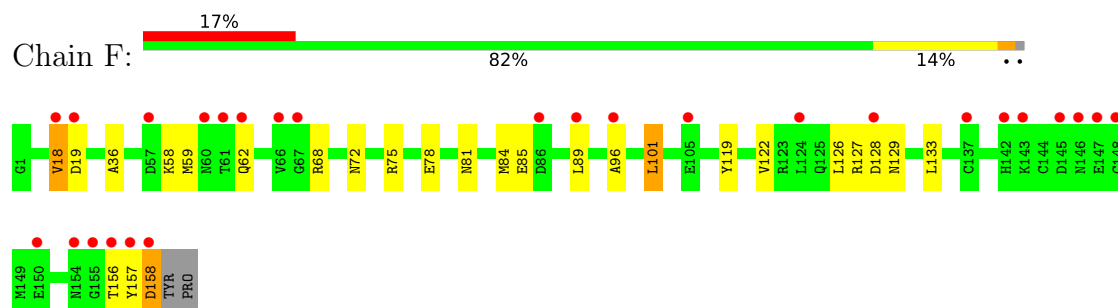
3 Residue-property plots [i](#)

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.

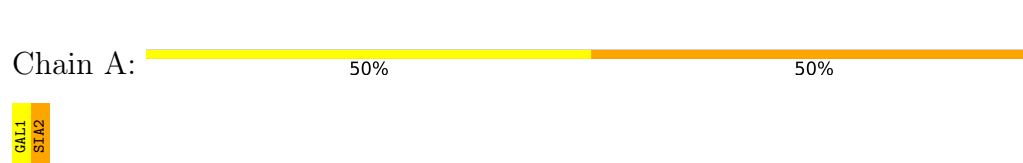
• Molecule 1: HAEMAGGLUTININ



• Molecule 2: HAEMAGGLUTININ



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	101.39Å 101.39Å 450.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.60) 98.4 (30.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.223 , (Not available) 0.246 , 0.266	Depositor DCC
R_{free} test set	1438 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4007	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: GAL, SIA, 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	E	0.49	0/2610	0.82	4/3545 (0.1%)
2	F	0.55	0/1296	0.85	2/1742 (0.1%)
All	All	0.51	0/3906	0.83	6/5287 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	ARG	CB-CA-C	-8.16	107.16	116.63
1	E	261	VAL	N-CA-C	6.35	116.50	110.53
1	E	194	LEU	N-CA-C	5.92	117.53	111.14
1	E	24	MET	N-CA-C	5.85	117.73	111.36
2	F	127	ARG	CB-CA-C	-5.19	110.61	116.63
2	F	18	VAL	N-CA-C	-5.16	107.72	112.83

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	E	2548	0	2490	58	1
2	F	1272	0	1186	17	0
3	A	25	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	28	0	26	0	0
5	E	72	0	0	6	0
5	F	62	0	0	2	0
All	All	4007	0	3721	71	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 9.

All (71) 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:E:168:TYR:HD1	1:E:169:ASN:N	1.51	1.08
1:E:159:SER:O	1:E:196:GLN:OE1	1.83	0.97
1:E:57:ARG:O	5:E:2026:HOH:O	1.83	0.94
1:E:168:TYR:HD1	1:E:168:TYR:C	1.75	0.94
1:E:168:TYR:CD1	1:E:169:ASN:N	2.36	0.93
1:E:159:SER:C	1:E:196:GLN:OE1	2.17	0.88
1:E:120:ILE:HG22	1:E:168:TYR:CE2	2.09	0.87
1:E:120:ILE:HG22	1:E:168:TYR:HE2	1.40	0.85
1:E:168:TYR:CE1	1:E:169:ASN:O	2.30	0.84
1:E:168:TYR:C	1:E:168:TYR:CD1	2.51	0.83
1:E:168:TYR:HE1	1:E:169:ASN:O	1.62	0.81
1:E:299:HIS:HD2	1:E:301:LEU:H	1.30	0.80
2:F:19:ASP:HB3	2:F:36:ALA:HB2	1.66	0.78
1:E:72:ASP:O	1:E:75:ILE:HG12	1.86	0.76
1:E:110:SER:HB3	5:E:2042:HOH:O	1.84	0.75
1:E:168:TYR:CE1	1:E:169:ASN:C	2.67	0.72
1:E:128:SER:HB3	1:E:162:PRO:HG2	1.73	0.69
1:E:60:SER:OG	1:E:92:ASP:OD1	2.04	0.68
1:E:168:TYR:HE1	1:E:169:ASN:C	2.02	0.67
1:E:9:ILE:HD11	2:F:122:VAL:HG21	1.78	0.66
1:E:56:LEU:O	1:E:57:ARG:HB2	1.96	0.65
1:E:120:ILE:HB	1:E:168:TYR:HD2	1.62	0.65
1:E:169:ASN:C	1:E:169:ASN:OD1	2.39	0.65
1:E:92:ASP:O	5:E:2036:HOH:O	2.15	0.64
1:E:190:ASP:OD2	3:A:2:SIA:H92	1.99	0.63
1:E:170:ASN:OD1	1:E:172:ASN:ND2	2.26	0.62
1:E:120:ILE:HB	1:E:168:TYR:CD2	2.35	0.61
1:E:299:HIS:CD2	1:E:301:LEU:H	2.18	0.59
1:E:113:ASN:OD1	1:E:264:GLY:HA3	2.03	0.57
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:TYR:HE1	1:E:170:ASN:HA	1.68	0.57
1:E:120:ILE:CG2	1:E:168:TYR:CE2	2.87	0.55
1:E:173:GLN:NE2	1:E:173:GLN:HA	2.21	0.55
1:E:168:TYR:CD1	1:E:169:ASN:C	2.84	0.55
2:F:59:MET:HE3	2:F:96:ALA:HA	1.88	0.55
2:F:157:TYR:O	2:F:158:ASP:HB2	2.07	0.54
1:E:115:PHE:HE1	1:E:260:ILE:HG12	1.72	0.54
1:E:95:TYR:CD1	1:E:230:MET:HG2	2.44	0.53
2:F:156:THR:O	2:F:156:THR:HG22	2.08	0.52
1:E:168:TYR:CE1	1:E:170:ASN:HA	2.44	0.52
1:E:151:VAL:HB	1:E:252:ILE:HG22	1.91	0.52
1:E:20:VAL:HG21	1:E:318:ALA:HB2	1.93	0.51
1:E:164:ILE:O	1:E:246:GLU:HA	2.11	0.50
1:E:169:ASN:HA	1:E:242:ALA:HA	1.94	0.50
2:F:126:LEU:O	2:F:129:ASN:HB2	2.11	0.50
1:E:62:ALA:HB3	1:E:92:ASP:OD1	2.12	0.49
1:E:285:PRO:HD3	1:E:301:LEU:O	2.13	0.48
1:E:97:GLY:HA3	1:E:230:MET:O	2.14	0.48
1:E:309:TYR:HD2	2:F:89:LEU:HD22	1.77	0.48
1:E:58:ASP:HB3	1:E:90:VAL:HG22	1.94	0.48
2:F:19:ASP:HB2	5:F:2012:HOH:O	2.13	0.48
1:E:115:PHE:HE1	1:E:260:ILE:CG1	2.27	0.47
2:F:84:MET:HE2	2:F:85:GLU:HG2	1.97	0.46
2:F:75:ARG:NH1	2:F:78:GLU:OE1	2.47	0.45
1:E:291:SER:HB2	5:E:2021:HOH:O	2.17	0.45
1:E:9:ILE:HG13	2:F:119:TYR:HA	1.98	0.45
1:E:120:ILE:HD11	1:E:254:PRO:HB2	2.00	0.44
1:E:129:HIS:HE1	5:E:2050:HOH:O	2.00	0.44
1:E:324:SER:HA	5:E:2069:HOH:O	2.18	0.44
2:F:72:ASN:HD22	2:F:75:ARG:HH21	1.65	0.44
1:E:169:ASN:HB2	1:E:242:ALA:HB2	2.00	0.43
1:E:203:SER:OG	1:E:246:GLU:HB3	2.18	0.43
2:F:72:ASN:ND2	2:F:75:ARG:HH21	2.17	0.43
2:F:101:LEU:HD13	5:F:2035:HOH:O	2.19	0.43
2:F:68:ARG:NH1	2:F:81:ASN:OD1	2.52	0.43
2:F:126:LEU:N	2:F:126:LEU:HD23	2.33	0.42
1:E:297:ASN:C	1:E:297:ASN:HD22	2.27	0.42
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.88	0.41
1:E:115:PHE:CE1	1:E:260:ILE:HG12	2.54	0.41
1:E:168:TYR:HD1	1:E:169:ASN:CA	2.26	0.40
1:E:295:PHE:HE1	2:F:62:GLN:OE1	2.05	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:E:259:LYS:NZ	1:E:262:LYS:NZ[11_565]	1.65	0.55

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	E	319/340 (94%)	306 (96%)	12 (4%)	1 (0%)	36	58
2	F	156/160 (98%)	153 (98%)	3 (2%)	0	100	100
All	All	475/500 (95%)	459 (97%)	15 (3%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	198	PRO

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	E	289/307 (94%)	272 (94%)	17 (6%)	18	38
2	F	134/136 (98%)	128 (96%)	6 (4%)	24	50
All	All	423/443 (96%)	400 (95%)	23 (5%)	20	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	49	ASP
1	E	70	MET
1	E	75	ILE
1	E	168	TYR
1	E	169	ASN
1	E	196	GLN
1	E	220	ARG
1	E	226	GLN
1	E	236	ILE
1	E	262	LYS
1	E	263	LYS
1	E	274	GLU
1	E	284	THR
1	E	297	ASN
1	E	301	LEU
1	E	315	LEU
1	E	321	LEU
2	F	18	VAL
2	F	58	LYS
2	F	101	LEU
2	F	128	ASP
2	F	133	LEU
2	F	158	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	19	GLN
1	E	91	ASN
1	E	119	GLN
1	E	173	GLN
1	E	211	GLN
1	E	226	GLN
1	E	297	ASN
1	E	299	HIS
2	F	25	HIS
2	F	26	HIS
2	F	42	GLN
2	F	62	GLN
2	F	72	ASN
2	F	125	GLN

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Mol	Chain	Res	Type
2	F	146	ASN
2	F	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GAL	A	1	3	4,4,12	0.54	0	4,4,17	1.37	1 (25%)
3	SIA	A	2	3	20,20,21	0.72	0	21,28,31	1.11	1 (4%)

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	GAL	A	1	3	-	1/2/2/22	-
3	SIA	A	2	3	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	SIA	O6-C2-C1	2.35	112.14	107.72
3	A	1	GAL	O2-C2-C3	-2.16	104.38	114.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

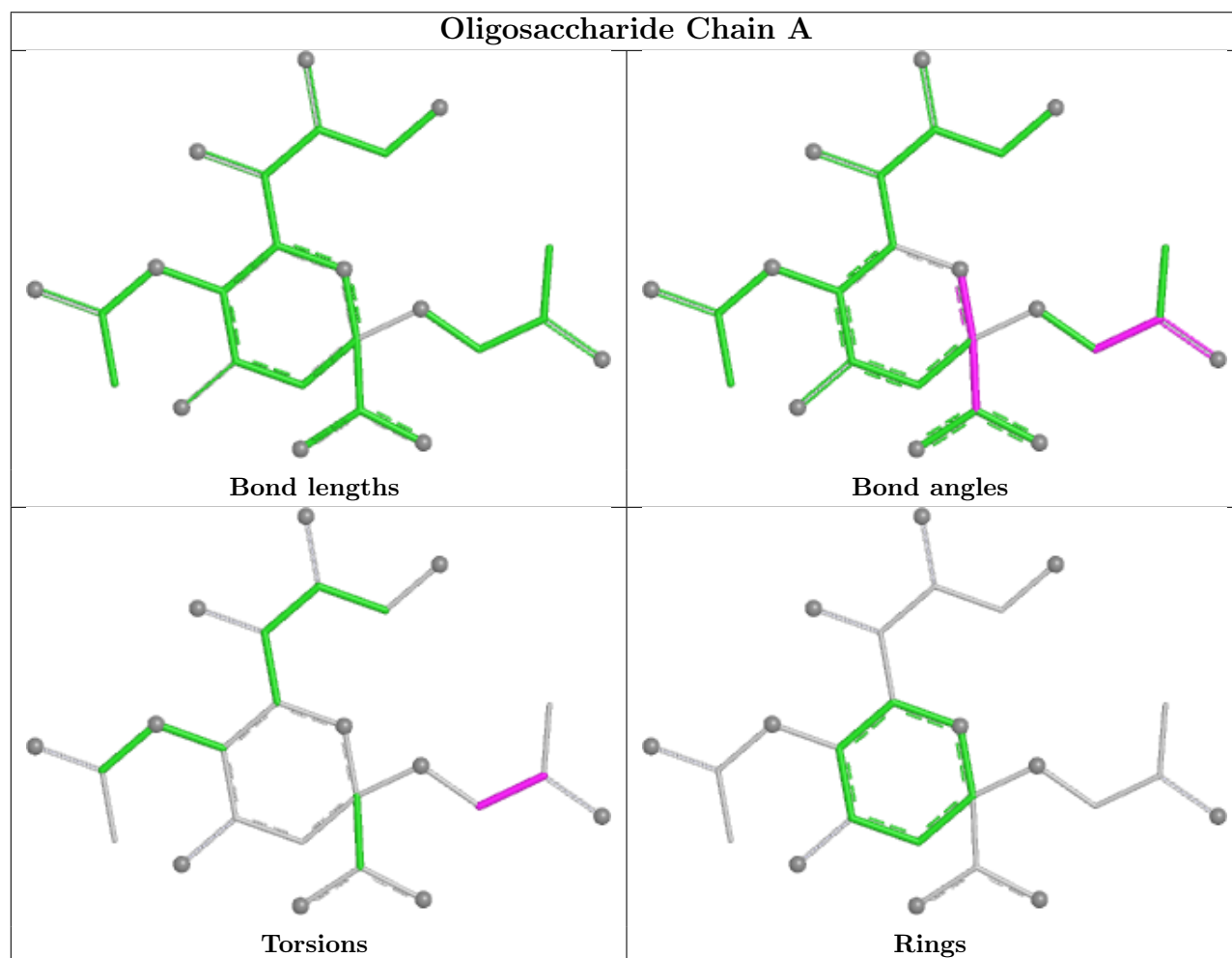
Mol	Chain	Res	Type	Atoms
3	A	1	GAL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	SIA	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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	F	411	1	14,14,15	0.41	0	17,19,21	0.67	0
4	NAG	F	421	1	14,14,15	0.44	0	17,19,21	1.01	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	411	1	-	2/6/23/26	0/1/1/1
4	NAG	F	421	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	421	NAG	C4-C3-C2	-2.02	108.06	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	411	NAG	O5-C5-C6-O6
4	F	411	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	E	321/340 (94%)	1.60	114 (35%)  	26, 70, 95, 100	0
2	F	158/160 (98%)	0.94	27 (17%)  	15, 45, 71, 95	0
All	All	479/500 (95%)	1.38	141 (29%)  	15, 61, 93, 100	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	173	GLN	6.3
2	F	60	ASN	5.8
1	E	278	CYS	5.8
1	E	155	ILE	5.5
1	E	171	THR	5.5
2	F	57	ASP	4.9
1	E	325	PRO	4.6
2	F	154	ASN	4.5
1	E	313	ASN	4.5
2	F	158	ASP	4.5
2	F	150	GLU	4.4
1	E	167	SER	4.1
1	E	59	CYS	4.0
1	E	172	ASN	4.0
1	E	161	TYR	3.9
1	E	139	CYS	3.9
1	E	127	SER	3.9
1	E	255	GLU	3.7
1	E	50	GLY	3.7
1	E	306	CYS	3.7
1	E	197	ASN	3.7
2	F	156	THR	3.6
1	E	169	ASN	3.6
1	E	49	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	98	ASP	3.5
1	E	305	GLU	3.5
1	E	51	VAL	3.5
1	E	131	ALA	3.4
1	E	124	SER	3.4
1	E	222	LYS	3.4
2	F	61	THR	3.4
1	E	186	ASN	3.4
2	F	142	HIS	3.4
2	F	128	ASP	3.4
1	E	118	ILE	3.3
1	E	188	ALA	3.3
1	E	219	THR	3.2
1	E	75	ILE	3.2
1	E	94	CYS	3.2
1	E	92	ASP	3.1
1	E	119	GLN	3.1
1	E	256	TYR	3.1
1	E	121	ILE	3.0
1	E	71	CYS	3.0
1	E	130	GLU	3.0
1	E	239	PRO	3.0
1	E	158	ASN	3.0
1	E	117	LYS	2.9
1	E	168	TYR	2.9
2	F	62	GLN	2.9
2	F	89	LEU	2.9
2	F	146	ASN	2.8
1	E	252	ILE	2.8
2	F	147	GLU	2.8
1	E	156	LYS	2.8
2	F	124	LEU	2.8
1	E	129	HIS	2.8
1	E	114	HIS	2.8
1	E	77	VAL	2.8
1	E	17	THR	2.7
1	E	191	GLN	2.7
1	E	190	ASP	2.7
1	E	195	TYR	2.7
1	E	160	THR	2.7
1	E	199	THR	2.7
1	E	175	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	198	PRO	2.7
2	F	148	CYS	2.6
1	E	170	ASN	2.6
1	E	120	ILE	2.6
1	E	243	ILE	2.6
1	E	261	VAL	2.6
1	E	148	PHE	2.6
1	E	324	SER	2.6
1	E	262	LYS	2.6
1	E	242	ALA	2.6
2	F	105	GLU	2.5
2	F	67	GLY	2.5
1	E	47	ASP	2.5
2	F	86	ASP	2.5
1	E	133	LEU	2.5
1	E	260	ILE	2.5
1	E	154	LEU	2.5
1	E	314	ARG	2.5
1	E	192	THR	2.5
1	E	264	GLY	2.5
1	E	254	PRO	2.5
1	E	147	PHE	2.5
1	E	42	ASN	2.4
1	E	274	GLU	2.4
1	E	44	LYS	2.4
2	F	66	VAL	2.4
1	E	174	GLU	2.4
1	E	57	ARG	2.4
2	F	157	TYR	2.3
1	E	244	ASN	2.3
1	E	144	LYS	2.3
1	E	203	SER	2.3
2	F	155	GLY	2.3
1	E	213	LEU	2.3
1	E	165	LYS	2.3
1	E	187	ASP	2.3
1	E	185	PRO	2.3
1	E	281	LYS	2.3
2	F	145	ASP	2.3
1	E	216	ARG	2.3
1	E	163	THR	2.3
1	E	166	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	217	ILE	2.2
1	E	299	HIS	2.2
1	E	279	ASN	2.2
1	E	152	VAL	2.2
1	E	116	GLU	2.2
1	E	128	SER	2.2
1	E	55	ILE	2.2
1	E	240	ASN	2.2
1	E	223	VAL	2.2
1	E	115	PHE	2.2
1	E	138	ALA	2.1
1	E	78	PRO	2.1
1	E	230	MET	2.1
1	E	301	LEU	2.1
1	E	227	SER	2.1
1	E	196	GLN	2.1
2	F	137	CYS	2.1
1	E	164	ILE	2.1
1	E	247	SER	2.1
1	E	194	LEU	2.1
1	E	143	GLY	2.1
1	E	80	TRP	2.1
1	E	123	LYS	2.0
1	E	134	GLY	2.0
1	E	135	VAL	2.0
1	E	218	ALA	2.0
1	E	257	ALA	2.0
2	F	19	ASP	2.0
2	F	96	ALA	2.0
2	F	143	LYS	2.0
1	E	126	TRP	2.0
1	E	153	TRP	2.0
2	F	18	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

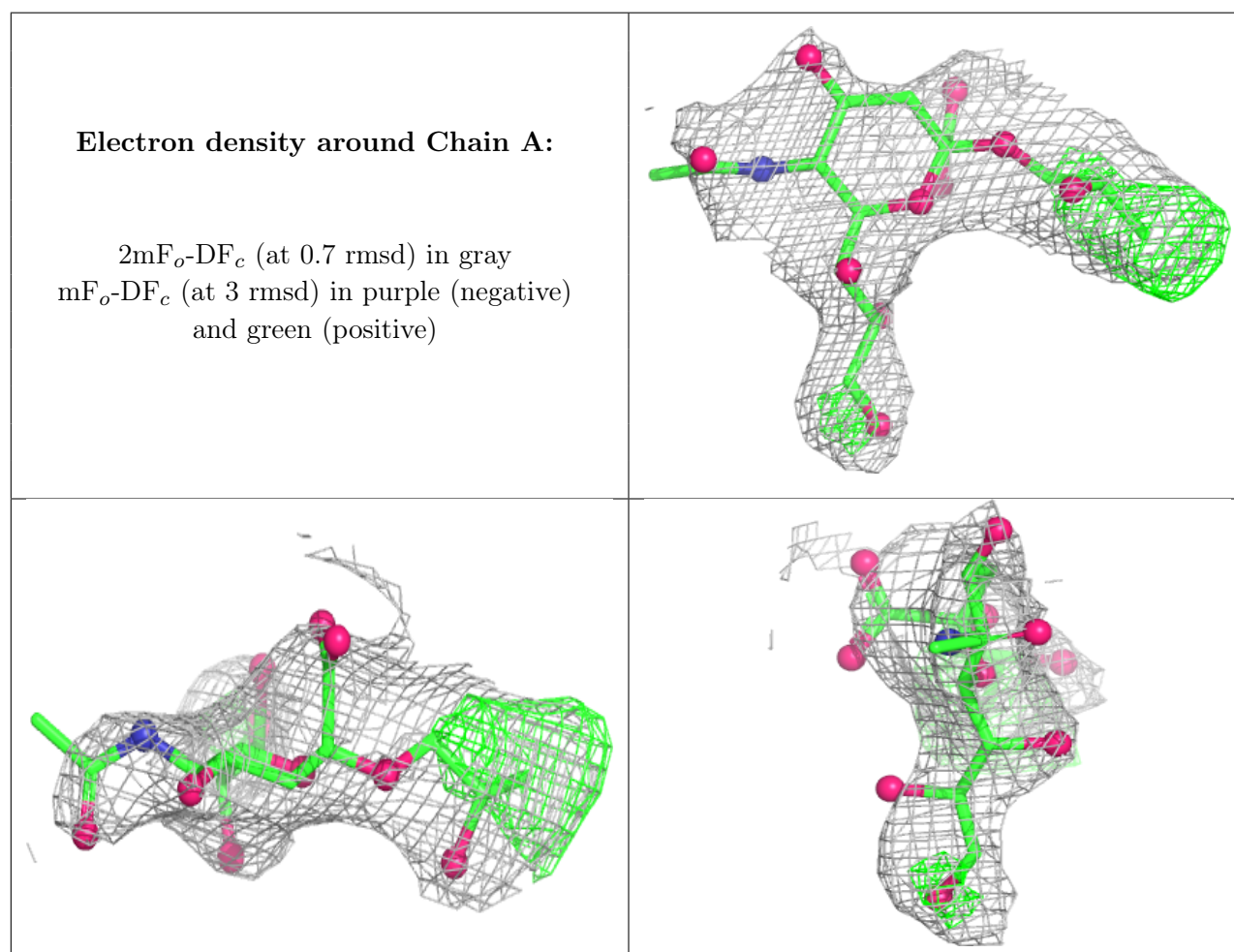
There are no non-standard protein/DNA/RNA residues in this entry.

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	GAL	A	1	5/12	-	-	130,130,131,131	0
3	SIA	A	2	20/21	-	-	130,130,130,130	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	411	14/15	0.72	0.17	79,80,80,80	0
4	NAG	F	421	14/15	0.73	0.17	73,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.