



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 AM UTC

PDB ID : 5TG8 / pdb_00005tg8
Title : Crystal structure of H15 hemagglutinin from A/shearwater/WA/2576/1979 H15N9 influenza virus
Authors : Wilson, I.A.; Tzarum, N.
Deposited on : 2016-09-27
Resolution : 3.10 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

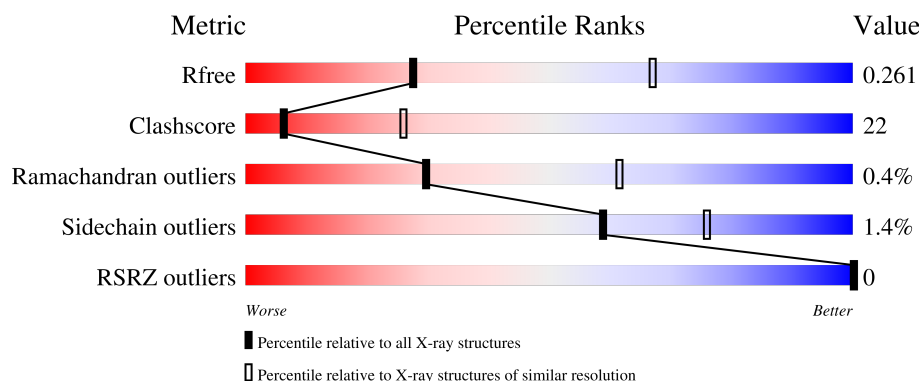
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	332	
1	C	332	
2	B	193	
2	D	193	
3	E	2	

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Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7874 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2514	1567	445	488	14			
1	C	328	Total	C	N	O	S	0	0	0
			2514	1567	445	488	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP L0L3X3
A	8	ASP	-	expression tag	UNP L0L3X3
A	9	PRO	-	expression tag	UNP L0L3X3
A	10	GLY	-	expression tag	UNP L0L3X3
C	7	ALA	-	expression tag	UNP L0L3X3
C	8	ASP	-	expression tag	UNP L0L3X3
C	9	PRO	-	expression tag	UNP L0L3X3
C	10	GLY	-	expression tag	UNP L0L3X3

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1381	850	247	277	7			
2	D	169	Total	C	N	O	S	0	0	0
			1381	850	247	277	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP L0L3X3
B	178	GLY	-	expression tag	UNP L0L3X3
B	179	GLY	-	expression tag	UNP L0L3X3
B	180	GLY	-	expression tag	UNP L0L3X3

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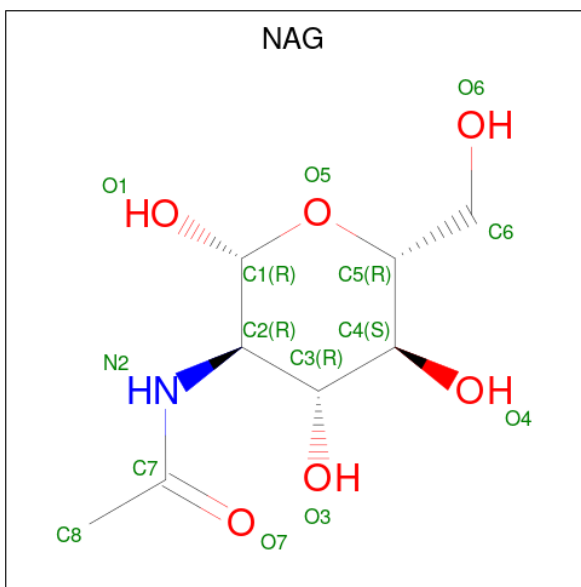
Chain	Residue	Modelled	Actual	Comment	Reference
B	181	GLY	-	expression tag	UNP L0L3X3
B	182	LEU	-	expression tag	UNP L0L3X3
B	183	ASN	-	expression tag	UNP L0L3X3
B	184	ASP	-	expression tag	UNP L0L3X3
B	185	ILE	-	expression tag	UNP L0L3X3
B	186	PHE	-	expression tag	UNP L0L3X3
B	187	GLU	-	expression tag	UNP L0L3X3
B	188	ALA	-	expression tag	UNP L0L3X3
B	189	GLN	-	expression tag	UNP L0L3X3
B	190	LYS	-	expression tag	UNP L0L3X3
D	177	SER	-	expression tag	UNP L0L3X3
D	178	GLY	-	expression tag	UNP L0L3X3
D	179	GLY	-	expression tag	UNP L0L3X3
D	180	GLY	-	expression tag	UNP L0L3X3
D	181	GLY	-	expression tag	UNP L0L3X3
D	182	LEU	-	expression tag	UNP L0L3X3
D	183	ASN	-	expression tag	UNP L0L3X3
D	184	ASP	-	expression tag	UNP L0L3X3
D	185	ILE	-	expression tag	UNP L0L3X3
D	186	PHE	-	expression tag	UNP L0L3X3
D	187	GLU	-	expression tag	UNP L0L3X3
D	188	ALA	-	expression tag	UNP L0L3X3
D	189	GLN	-	expression tag	UNP L0L3X3
D	190	LYS	-	expression tag	UNP L0L3X3

- Molecule 3 is an oligosaccharide called 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	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

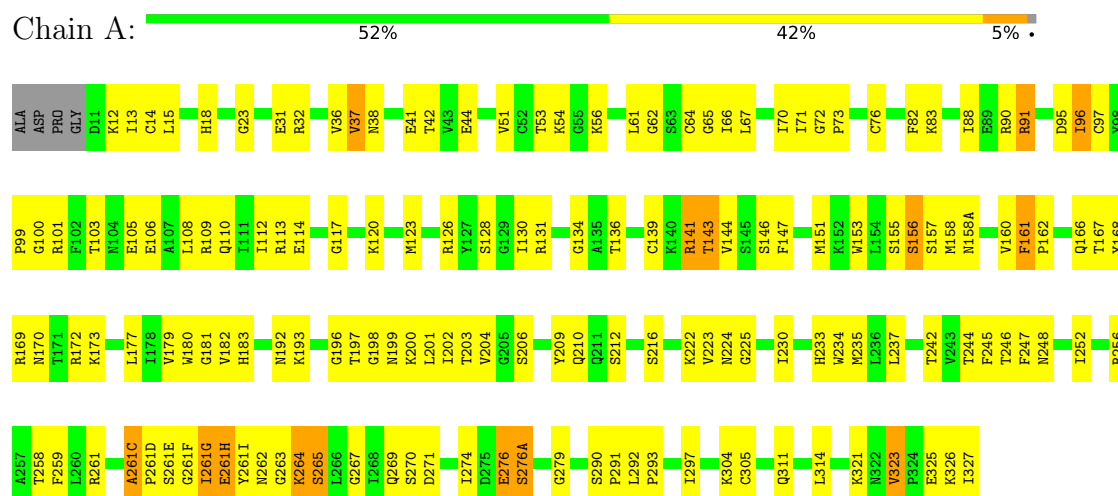


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

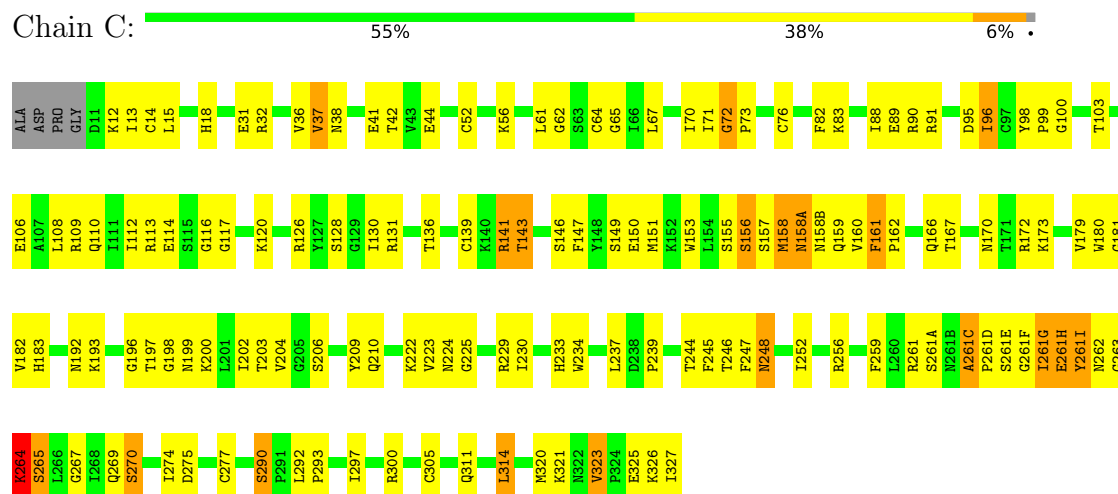
3 Residue-property plots

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: Hemagglutinin HA1 chain

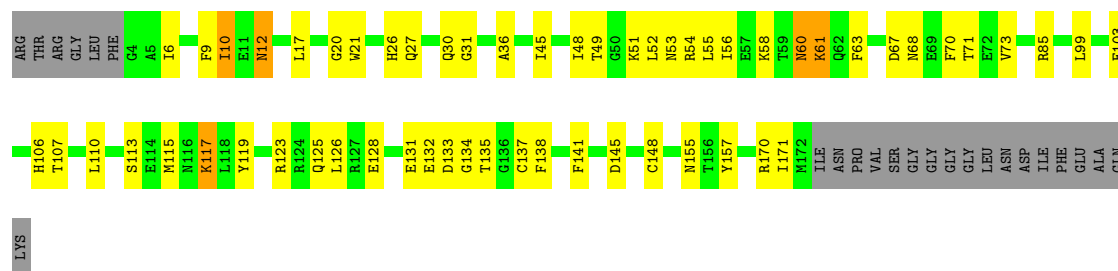


• Molecule 1: Hemagglutinin HA1 chain



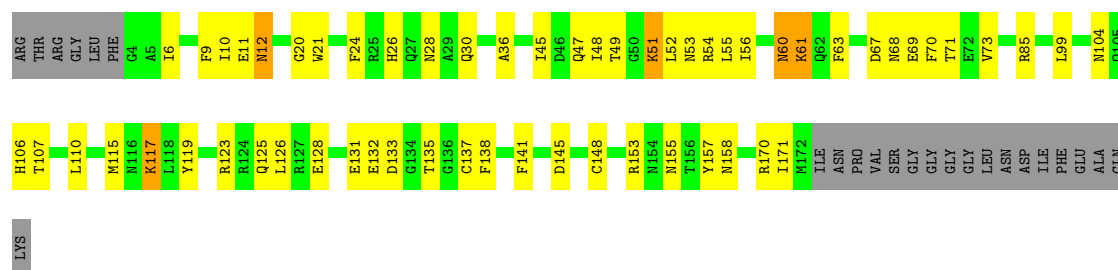
• Molecule 2: Hemagglutinin HA2 chain





- Molecule 2: Hemagglutinin HA2 chain

Chain D: 57% 28% 12%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	115.99Å 115.99Å 128.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.39 – 3.10 39.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.39-3.10) 93.7 (39.39-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.222 , 0.262 0.223 , 0.261	Depositor DCC
R_{free} test set	1780 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 11.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.440 for -h,-k,l 0.048 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7874	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: 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	0.75	1/2563 (0.0%)	1.31	25/3463 (0.7%)
1	C	0.75	1/2563 (0.0%)	1.37	28/3463 (0.8%)
2	B	0.94	1/1404 (0.1%)	1.14	6/1894 (0.3%)
2	D	0.91	0/1404	1.15	7/1894 (0.4%)
All	All	0.82	3/7934 (0.0%)	1.27	66/10714 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	THR	CA-CB	6.26	1.64	1.53
1	A	143	THR	CA-CB	5.29	1.62	1.53
2	B	10	ILE	CA-C	-5.01	1.46	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	LYS	N-CA-C	20.48	138.93	111.28
1	A	263	GLY	N-CA-C	15.25	131.81	112.14
1	A	261(H)	GLU	N-CA-C	-13.86	95.79	113.12
1	C	261(H)	GLU	N-CA-C	-13.84	95.81	113.12
1	C	264	LYS	CB-CA-C	-12.90	93.27	112.11
1	A	264	LYS	N-CA-C	12.79	128.89	111.24
1	C	265	SER	N-CA-C	12.49	127.01	110.53
1	A	297	ILE	N-CA-C	10.83	120.71	110.53
1	C	297	ILE	N-CA-C	10.45	120.36	110.53
1	C	161	PHE	CA-C-N	9.73	129.78	119.76
1	C	161	PHE	C-N-CA	9.73	129.78	119.76
1	A	161	PHE	CA-C-N	9.68	130.29	119.83
1	A	161	PHE	C-N-CA	9.68	130.29	119.83
1	A	261(C)	ALA	C-N-CD	-9.13	100.52	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	261(C)	ALA	C-N-CD	-9.11	100.55	120.60
1	A	72	GLY	N-CA-C	8.57	129.83	112.34
2	D	53	ASN	N-CA-C	-8.40	103.55	113.88
1	C	265	SER	N-CA-CB	-8.39	98.36	110.36
1	C	72	GLY	N-CA-C	8.26	129.19	112.34
2	B	53	ASN	N-CA-C	-8.05	103.98	113.88
1	C	263	GLY	N-CA-C	7.97	132.06	113.18
1	C	91	ARG	N-CA-C	7.72	119.78	111.36
1	C	12	LYS	N-CA-C	7.69	122.00	109.85
1	A	91	ARG	N-CA-C	7.48	119.22	111.14
1	A	12	LYS	N-CA-C	6.97	120.87	109.85
1	C	65	GLY	N-CA-C	-6.93	103.67	112.54
1	A	265	SER	N-CA-C	6.89	119.63	110.53
1	C	56	LYS	N-CA-C	-6.84	98.69	109.50
1	A	305	CYS	N-CA-C	6.66	120.29	110.10
1	A	23	GLY	N-CA-C	6.61	119.53	111.93
1	C	323	VAL	CA-C-N	6.61	126.65	119.90
1	C	323	VAL	C-N-CA	6.61	126.65	119.90
1	A	65	GLY	N-CA-C	-6.49	104.23	112.54
1	C	305	CYS	N-CA-C	6.28	119.71	110.10
2	B	117	LYS	N-CA-C	-6.26	104.37	111.07
1	A	314	LEU	CA-C-N	-6.08	112.25	119.84
1	A	314	LEU	C-N-CA	-6.08	112.25	119.84
1	A	128	SER	N-CA-C	5.93	120.32	111.96
1	C	261(I)	TYR	CB-CA-C	5.86	117.00	109.80
2	B	171	ILE	N-CA-C	5.79	116.43	110.82
1	A	96	ILE	N-CA-C	5.71	116.70	108.48
1	C	156	SER	N-CA-C	5.68	119.31	112.38
1	C	128	SER	N-CA-C	5.65	119.93	111.96
2	D	171	ILE	N-CA-C	5.61	116.26	110.82
1	C	311	GLN	N-CA-C	5.57	118.31	109.96
2	D	12	ASN	N-CA-C	5.54	117.49	109.07
1	C	96	ILE	N-CA-C	5.53	116.45	108.48
2	D	60	ASN	N-CA-C	5.50	118.44	109.59
1	C	37	VAL	N-CA-C	5.45	115.66	110.53
1	A	311	GLN	N-CA-C	5.42	118.09	109.96
1	A	323	VAL	CA-C-N	5.42	125.43	119.90
1	A	323	VAL	C-N-CA	5.42	125.43	119.90
2	B	60	ASN	N-CA-C	5.38	118.25	109.59
1	A	37	VAL	N-CA-C	5.36	116.14	110.72
2	B	12	ASN	N-CA-C	5.36	117.33	109.24
1	A	156	SER	N-CA-C	5.29	118.84	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	LYS	N-CA-C	-5.27	107.50	114.04
2	D	51	LYS	N-CA-C	-5.22	102.55	110.28
2	D	104	ASN	N-CA-C	5.21	117.04	111.36
1	A	216	SER	CA-C-N	5.15	125.31	119.90
1	A	216	SER	C-N-CA	5.15	125.31	119.90
1	C	270	SER	N-CA-C	5.09	117.12	109.23
1	C	314	LEU	CA-C-N	-5.07	113.50	119.84
1	C	314	LEU	C-N-CA	-5.07	113.50	119.84
1	C	290	SER	N-CA-C	5.04	114.61	108.11
2	D	117	LYS	N-CA-C	-5.04	105.67	111.07

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	2514	0	2471	121	0
1	C	2514	0	2473	121	0
2	B	1381	0	1287	63	0
2	D	1381	0	1287	65	0
3	E	28	0	25	2	0
3	F	28	0	25	3	0
4	B	14	0	13	0	0
4	D	14	0	13	1	0
All	All	7874	0	7594	342	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 22.

All (342) 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:C:18:HIS:HD2	2:D:21:TRP:HA	1.12	1.13
2:D:9:PHE:CE2	2:D:10:ILE:HD13	1.85	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:HIS:HD2	2:B:21:TRP:HA	1.22	1.02
1:C:38:ASN:ND2	3:F:1:NAG:O7	1.99	0.96
1:A:38:ASN:ND2	3:E:1:NAG:O7	2.00	0.94
1:C:18:HIS:CD2	2:D:21:TRP:HA	2.03	0.93
1:C:300:ARG:NH1	2:D:69:GLU:HG3	1.85	0.92
2:B:9:PHE:CE2	2:B:10:ILE:HD13	2.04	0.92
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.08	0.87
2:D:51:LYS:HG2	2:D:54:ARG:HH12	1.41	0.86
1:A:261:ARG:NH1	1:A:261(H):GLU:HG3	1.91	0.85
1:C:131:ARG:HG3	1:C:157:SER:HA	1.57	0.84
2:D:61:LYS:NZ	2:D:63:PHE:HB2	1.94	0.82
1:C:326:LYS:H	2:D:12:ASN:HD21	1.25	0.82
1:A:326:LYS:H	2:B:12:ASN:HD21	1.28	0.82
1:C:113:ARG:O	1:C:265:SER:OG	1.97	0.82
1:C:261:ARG:NH1	1:C:261(H):GLU:HG3	1.95	0.80
1:A:131:ARG:HG3	1:A:157:SER:HA	1.63	0.80
1:A:18:HIS:HE1	1:A:37:VAL:HG11	1.46	0.79
1:A:261(F):GLY:O	1:A:261(G):ILE:HG13	1.82	0.79
1:C:261(F):GLY:O	1:C:261(G):ILE:HG13	1.82	0.79
1:C:131:ARG:HB2	1:C:155:SER:HB2	1.67	0.76
1:C:300:ARG:HH12	2:D:69:GLU:HG3	1.47	0.76
2:D:61:LYS:HZ3	2:D:63:PHE:HB2	1.49	0.76
1:A:71:ILE:HG22	1:A:151:MET:HE3	1.66	0.76
1:C:166:GLN:HB2	1:C:245:PHE:HB2	1.67	0.76
2:B:128:GLU:HG3	2:B:170:ARG:HH12	1.50	0.75
1:C:170:ASN:HB2	1:C:237:LEU:HD23	1.67	0.74
1:A:170:ASN:HB2	1:A:237:LEU:HD23	1.68	0.74
1:A:222:LYS:HE2	1:A:225:GLY:HA2	1.69	0.74
1:A:327:ILE:HD12	1:A:327:ILE:H	1.52	0.73
1:A:131:ARG:HB2	1:A:155:SER:HB2	1.72	0.72
1:C:71:ILE:HG22	1:C:151:MET:HE3	1.72	0.71
1:A:141:ARG:O	1:A:143:THR:HG22	1.91	0.71
1:C:325:GLU:HA	2:D:12:ASN:OD1	1.91	0.70
1:A:90:ARG:NH1	1:A:270:SER:O	2.24	0.70
1:C:120:LYS:HB2	1:C:256:ARG:HH21	1.56	0.69
2:D:133:ASP:OD2	2:D:137:CYS:HB2	1.91	0.69
1:C:41:GLU:O	1:C:292:LEU:CD2	2.41	0.69
2:D:9:PHE:CE2	2:D:10:ILE:CD1	2.70	0.69
2:D:145:ASP:H	2:D:148:CYS:HB3	1.58	0.69
1:A:41:GLU:O	1:A:292:LEU:CD2	2.41	0.69
1:C:41:GLU:O	1:C:292:LEU:HD22	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:LEU:HD23	2:B:99:LEU:HD23	1.74	0.68
1:C:160:VAL:HA	1:C:196:GLY:HA3	1.76	0.68
1:A:41:GLU:O	1:A:292:LEU:HD22	1.94	0.68
1:C:327:ILE:HD12	1:C:327:ILE:H	1.58	0.68
1:A:136:THR:HG23	1:A:139:CYS:H	1.58	0.68
1:C:141:ARG:O	1:C:143:THR:HG22	1.93	0.67
1:C:18:HIS:HE1	1:C:37:VAL:HG11	1.59	0.67
1:C:136:THR:HG23	1:C:139:CYS:H	1.58	0.67
1:A:325:GLU:HA	2:B:12:ASN:OD1	1.94	0.67
1:A:96:ILE:HD13	1:A:99:PRO:HA	1.78	0.66
1:A:200:LYS:HA	1:A:248:ASN:ND2	2.11	0.66
2:D:9:PHE:CZ	2:D:10:ILE:CD1	2.79	0.66
2:B:141:PHE:CG	2:B:170:ARG:HG3	2.30	0.66
1:C:206:SER:HB3	1:C:209:TYR:HB3	1.78	0.66
2:D:141:PHE:CG	2:D:170:ARG:HG3	2.31	0.66
2:D:9:PHE:CZ	2:D:10:ILE:HD13	2.30	0.65
1:A:261:ARG:HH12	1:A:261(H):GLU:HG3	1.60	0.65
2:D:55:LEU:HD23	2:D:99:LEU:HD23	1.78	0.65
1:A:200:LYS:HA	1:A:248:ASN:HD21	1.61	0.65
1:A:180:TRP:CE2	1:A:233:HIS:HB2	2.32	0.64
1:A:202:ILE:HG23	1:A:247:PHE:HB3	1.79	0.64
2:B:61:LYS:NZ	2:B:63:PHE:HB2	2.13	0.63
2:B:131:GLU:HG3	2:B:141:PHE:CE1	2.34	0.63
1:A:170:ASN:ND2	1:A:237:LEU:O	2.32	0.62
1:A:42:THR:HA	1:A:292:LEU:HD22	1.82	0.62
1:C:264:LYS:O	1:C:264:LYS:HG3	1.99	0.62
1:C:200:LYS:HA	1:C:248:ASN:ND2	2.15	0.62
2:D:128:GLU:HG3	2:D:170:ARG:HH12	1.64	0.61
2:D:51:LYS:HD3	2:D:54:ARG:NH1	2.15	0.61
1:A:160:VAL:HA	1:A:196:GLY:HA3	1.83	0.61
1:A:120:LYS:HB2	1:A:256:ARG:HH21	1.65	0.61
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.66	0.61
1:C:172:ARG:HD3	1:C:259:PHE:CZ	2.36	0.61
1:C:100:GLY:HA3	1:C:230:ILE:O	2.01	0.61
1:A:71:ILE:CG2	1:A:151:MET:HE3	2.31	0.60
2:B:145:ASP:H	2:B:148:CYS:HB3	1.66	0.60
2:D:51:LYS:CG	2:D:54:ARG:HH12	2.14	0.60
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.37	0.60
1:A:100:GLY:HA3	1:A:230:ILE:O	2.02	0.60
1:A:130:ILE:HG23	1:A:155:SER:O	2.02	0.60
2:D:52:LEU:H	2:D:55:LEU:HD12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ILE:HG23	1:C:155:SER:O	2.02	0.59
1:C:180:TRP:CE2	1:C:233:HIS:HB2	2.37	0.59
1:C:222:LYS:HE2	1:C:225:GLY:HA2	1.84	0.59
1:C:261(D):PRO:O	1:C:261(E):SER:HB2	2.02	0.59
2:B:131:GLU:HG3	2:B:141:PHE:HE1	1.67	0.59
1:C:103:THR:HG22	1:C:233:HIS:HA	1.85	0.59
2:D:125:GLN:HE22	2:D:155:ASN:HA	1.68	0.59
1:C:13:ILE:HG22	2:D:138:PHE:HB2	1.85	0.58
1:C:52:CYS:CB	1:C:277:CYS:HG	2.14	0.58
1:C:96:ILE:HD13	1:C:99:PRO:HA	1.85	0.58
1:C:261(C):ALA:HB3	1:C:261(I):TYR:HB2	1.85	0.58
2:B:51:LYS:HG2	2:B:54:ARG:HH12	1.68	0.58
1:C:52:CYS:HG	1:C:277:CYS:HG	0.62	0.58
1:C:106:GLU:HG2	2:D:73:VAL:HG12	1.86	0.57
1:A:97:CYS:O	1:A:224:ASN:ND2	2.35	0.57
1:A:261(D):PRO:O	1:A:261(E):SER:HB2	2.02	0.57
2:D:131:GLU:HG3	2:D:141:PHE:CE1	2.38	0.57
1:A:70:ILE:HG21	1:A:179:VAL:HG21	1.85	0.57
1:A:261(C):ALA:HB3	1:A:261(I):TYR:HB2	1.86	0.57
1:C:44:GLU:HG2	1:C:290:SER:HB2	1.87	0.57
1:C:261:ARG:HH12	1:C:261(H):GLU:HG3	1.70	0.57
2:D:123:ARG:HD3	2:D:132:GLU:OE2	2.05	0.57
1:A:261(G):ILE:HD12	1:A:261(G):ILE:O	2.06	0.56
1:A:103:THR:HG22	1:A:233:HIS:HA	1.87	0.56
1:A:206:SER:HB3	1:A:209:TYR:HB3	1.87	0.56
2:D:145:ASP:O	2:D:148:CYS:N	2.37	0.56
1:C:261(G):ILE:O	1:C:261(G):ILE:HD12	2.06	0.56
2:D:133:ASP:CG	2:D:137:CYS:HB2	2.30	0.56
1:C:42:THR:HA	1:C:292:LEU:HD22	1.87	0.55
1:C:153:TRP:HZ2	1:C:183:HIS:CE1	2.24	0.55
2:B:51:LYS:HE3	2:B:103:GLU:HB3	1.87	0.55
2:D:20:GLY:HA3	2:D:36:ALA:HB1	1.88	0.55
2:D:48:ILE:HD11	2:D:107:THR:HG23	1.89	0.55
1:A:18:HIS:CE1	1:A:37:VAL:HG11	2.35	0.55
1:C:181:GLY:HA3	1:C:252:ILE:HB	1.90	0.54
2:B:9:PHE:CE2	2:B:10:ILE:CD1	2.84	0.54
2:B:133:ASP:OD2	2:B:137:CYS:HB2	2.07	0.54
1:A:61:LEU:HB3	1:A:64:CYS:HB3	1.89	0.54
1:A:139:CYS:HB2	1:A:146:SER:O	2.07	0.54
2:B:61:LYS:HZ3	2:B:63:PHE:HB2	1.73	0.54
1:C:106:GLU:HG2	2:D:73:VAL:CG1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:O	1:A:210:GLN:HA	2.08	0.54
1:C:202:ILE:HG23	1:C:247:PHE:HB3	1.88	0.54
2:B:52:LEU:H	2:B:55:LEU:HD12	1.74	0.53
2:D:9:PHE:CZ	2:D:10:ILE:HD11	2.43	0.53
1:A:106:GLU:HG2	2:B:73:VAL:CG1	2.39	0.53
2:B:20:GLY:HA3	2:B:36:ALA:HB1	1.90	0.53
1:A:88:ILE:HD12	1:A:274:ILE:HD11	1.90	0.53
1:C:38:ASN:ND2	3:F:1:NAG:C7	2.72	0.53
1:C:204:VAL:O	1:C:210:GLN:HA	2.09	0.53
1:A:120:LYS:HB2	1:A:256:ARG:NH2	2.24	0.53
2:D:61:LYS:HZ1	2:D:63:PHE:HB2	1.72	0.53
1:C:42:THR:O	1:C:293:PRO:HD2	2.09	0.53
1:A:91:ARG:NH2	1:A:271:ASP:OD2	2.43	0.52
1:A:44:GLU:HG2	1:A:290:SER:HB2	1.92	0.52
1:A:113:ARG:HB3	1:A:267:GLY:HA3	1.92	0.52
1:A:276:GLU:HG3	2:D:30:GLN:O	2.09	0.52
1:A:15:LEU:HD22	2:B:119:TYR:HA	1.91	0.52
1:A:106:GLU:HG2	2:B:73:VAL:HG12	1.92	0.52
2:B:133:ASP:CG	2:B:137:CYS:HB2	2.35	0.51
2:D:141:PHE:CD2	2:D:170:ARG:HG3	2.45	0.51
1:A:42:THR:O	1:A:293:PRO:HD2	2.10	0.51
1:C:170:ASN:ND2	1:C:237:LEU:O	2.42	0.51
1:A:192:ASN:HA	1:A:196:GLY:O	2.10	0.51
1:A:13:ILE:HG22	2:B:138:PHE:HB2	1.91	0.51
1:C:158(A):ASN:OD1	1:C:193:LYS:HE2	2.09	0.51
1:C:192:ASN:HA	1:C:196:GLY:O	2.10	0.51
1:A:222:LYS:CE	1:A:225:GLY:HA2	2.39	0.51
2:B:26:HIS:ND1	2:B:26:HIS:C	2.69	0.51
1:C:61:LEU:HB3	1:C:64:CYS:HB3	1.91	0.51
1:A:156:SER:O	1:A:157:SER:OG	2.23	0.51
2:D:45:ILE:O	2:D:49:THR:HG23	2.10	0.51
1:C:139:CYS:O	1:C:146:SER:HB3	2.10	0.51
1:A:67:LEU:N	1:A:95:ASP:OD1	2.41	0.51
1:A:326:LYS:H	2:B:12:ASN:ND2	2.03	0.51
1:C:269:GLN:HB3	2:D:70:PHE:CE2	2.45	0.51
1:C:52:CYS:CB	1:C:277:CYS:SG	2.99	0.50
2:B:133:ASP:OD2	2:B:135:THR:OG1	2.28	0.50
2:B:123:ARG:HD3	2:B:132:GLU:OE2	2.11	0.50
1:A:139:CYS:O	1:A:146:SER:HB3	2.12	0.50
2:B:30:GLN:OE1	2:B:30:GLN:N	2.42	0.50
2:B:145:ASP:O	2:B:148:CYS:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:ASP:OD2	2:D:135:THR:OG1	2.30	0.50
2:B:51:LYS:HD3	2:B:54:ARG:NH1	2.26	0.50
1:C:90:ARG:NH1	1:C:270:SER:O	2.45	0.50
1:C:199:ASN:O	1:C:248:ASN:ND2	2.44	0.50
1:A:14:CYS:SG	2:B:6:ILE:HG13	2.52	0.50
2:D:131:GLU:HG3	2:D:141:PHE:HE1	1.77	0.50
1:A:38:ASN:ND2	3:E:1:NAG:C7	2.73	0.50
1:C:88:ILE:HD12	1:C:274:ILE:HD11	1.93	0.50
1:A:181:GLY:HA3	1:A:252:ILE:HB	1.93	0.49
1:C:114:GLU:HA	1:C:265:SER:O	2.12	0.49
1:C:67:LEU:N	1:C:95:ASP:OD1	2.45	0.49
1:C:120:LYS:HB2	1:C:256:ARG:NH2	2.25	0.49
2:B:17:LEU:HD11	2:B:36:ALA:HB2	1.94	0.49
1:C:139:CYS:HB2	1:C:146:SER:O	2.13	0.49
1:A:167:THR:HG22	1:A:244:THR:OG1	2.13	0.49
1:A:153:TRP:HZ2	1:A:183:HIS:CE1	2.31	0.48
1:A:41:GLU:O	1:A:292:LEU:HD21	2.12	0.48
1:C:15:LEU:HD22	2:D:119:TYR:HA	1.94	0.48
2:D:68:ASN:HB3	2:D:71:THR:O	2.13	0.48
1:A:117:GLY:C	1:A:261:ARG:HG3	2.38	0.48
2:D:128:GLU:O	2:D:170:ARG:NH1	2.46	0.48
1:A:70:ILE:HD11	1:A:112:ILE:HG13	1.95	0.48
1:C:31:GLU:HG2	1:C:32:ARG:H	1.78	0.48
2:D:56:ILE:HG23	2:D:60:ASN:OD1	2.14	0.48
1:C:41:GLU:O	1:C:292:LEU:HD21	2.12	0.48
2:D:26:HIS:HD2	2:D:153:ARG:HH21	1.61	0.48
2:B:128:GLU:O	2:B:170:ARG:NH1	2.47	0.48
1:C:14:CYS:SG	2:D:6:ILE:HG13	2.54	0.48
1:C:110:GLN:HA	1:C:113:ARG:HD2	1.96	0.48
1:A:44:GLU:HG2	1:A:290:SER:CB	2.43	0.48
2:B:56:ILE:HG23	2:B:60:ASN:OD1	2.14	0.47
1:C:167:THR:HG22	1:C:244:THR:OG1	2.14	0.47
2:B:68:ASN:HB3	2:B:71:THR:O	2.14	0.47
2:B:45:ILE:O	2:B:49:THR:HG23	2.14	0.47
2:B:52:LEU:HA	2:B:55:LEU:HD12	1.97	0.47
1:A:36:VAL:HG12	1:A:321:LYS:HA	1.95	0.47
1:A:292:LEU:HD23	2:B:52:LEU:HD11	1.96	0.47
1:A:67:LEU:HB2	1:A:95:ASP:OD1	2.14	0.47
1:C:36:VAL:HG12	1:C:321:LYS:HA	1.97	0.47
1:A:67:LEU:HG	1:A:109:ARG:HG2	1.97	0.47
1:A:161:PHE:HB3	1:A:248:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:GLU:HG3	2:B:170:ARG:NH1	2.25	0.47
1:C:113:ARG:HB3	1:C:267:GLY:HA3	1.97	0.47
2:D:51:LYS:O	2:D:52:LEU:HB3	2.15	0.47
1:C:160:VAL:HG22	1:C:197:THR:H	1.80	0.47
1:A:182:VAL:HG22	1:A:202:ILE:HD12	1.97	0.47
1:A:269:GLN:HB3	2:B:70:PHE:CE2	2.50	0.47
1:C:146:SER:OG	1:C:147:PHE:N	2.46	0.47
2:D:30:GLN:OE1	2:D:30:GLN:N	2.45	0.47
1:C:52:CYS:HB3	1:C:277:CYS:SG	2.55	0.46
1:C:206:SER:N	1:C:209:TYR:O	2.37	0.46
1:A:323:VAL:O	1:A:323:VAL:HG12	2.15	0.46
2:D:47:GLN:OE1	2:D:110:LEU:HD22	2.15	0.46
1:A:18:HIS:HD2	2:B:21:TRP:CA	2.08	0.46
1:C:67:LEU:HB2	1:C:95:ASP:OD1	2.16	0.46
1:A:180:TRP:NE1	1:A:233:HIS:HB2	2.31	0.46
2:B:26:HIS:C	2:B:26:HIS:HD1	2.24	0.46
2:B:141:PHE:CD2	2:B:170:ARG:HG3	2.50	0.46
1:C:70:ILE:HD11	1:C:112:ILE:HG13	1.97	0.46
1:C:117:GLY:C	1:C:261:ARG:HG3	2.41	0.46
1:A:62:GLY:HA2	1:A:90:ARG:HG3	1.98	0.45
1:C:70:ILE:HG21	1:C:179:VAL:HG21	1.97	0.45
1:A:51:VAL:HG12	1:A:53:THR:HG22	1.97	0.45
1:A:158(A):ASN:OD1	1:A:193:LYS:HE2	2.16	0.45
1:A:172:ARG:HD3	1:A:259:PHE:CE2	2.52	0.45
1:C:44:GLU:HG2	1:C:290:SER:CB	2.45	0.45
2:B:67:ASP:CG	2:B:85:ARG:HH22	2.25	0.45
2:B:133:ASP:OD1	2:B:134:GLY:N	2.49	0.45
1:C:158:MET:HE2	1:C:158:MET:HB3	1.72	0.45
1:A:166:GLN:HB2	1:A:245:PHE:HB2	1.98	0.45
1:A:177:LEU:HB3	1:A:258:THR:HB	1.98	0.45
1:A:200:LYS:HD3	1:A:248:ASN:ND2	2.31	0.45
1:C:108:LEU:HD22	1:C:234:TRP:CD1	2.52	0.45
1:C:166:GLN:O	1:C:244:THR:HA	2.17	0.45
1:A:108:LEU:HD13	1:A:234:TRP:CE3	2.52	0.45
1:C:200:LYS:HA	1:C:248:ASN:HD21	1.81	0.45
2:D:126:LEU:HD23	2:D:157:TYR:CE2	2.52	0.45
1:A:131:ARG:CG	1:A:157:SER:HA	2.41	0.45
2:D:67:ASP:OD1	2:D:67:ASP:N	2.50	0.45
2:D:106:HIS:NE2	2:D:110:LEU:HD23	2.32	0.45
1:A:173:LYS:N	1:A:173:LYS:HD2	2.32	0.44
2:B:48:ILE:HD11	2:B:107:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:HG2	1:A:32:ARG:H	1.83	0.44
1:A:54:LYS:HD2	1:A:276(A):SER:O	2.18	0.44
1:A:123:MET:HE3	1:A:168:TYR:CD2	2.52	0.44
1:C:73:PRO:HD2	1:C:76:CYS:HB2	2.00	0.44
1:C:131:ARG:CG	1:C:157:SER:HA	2.40	0.44
1:C:323:VAL:O	1:C:323:VAL:HG12	2.17	0.44
1:A:235:MET:HB2	1:A:235:MET:HE3	1.78	0.44
2:D:128:GLU:HG3	2:D:170:ARG:NH1	2.31	0.44
1:A:157:SER:O	1:A:158:MET:HG3	2.17	0.44
1:A:223:VAL:O	1:A:224:ASN:HB2	2.18	0.44
2:B:61:LYS:HZ1	2:B:63:PHE:HB2	1.83	0.44
1:C:275:ASP:OD2	1:C:277:CYS:CB	2.66	0.44
2:D:24:PHE:CD1	2:D:153:ARG:HD3	2.52	0.44
1:A:130:ILE:HG22	1:A:131:ARG:O	2.18	0.44
1:C:223:VAL:O	1:C:224:ASN:HB2	2.16	0.44
1:C:320:MET:HE2	1:C:320:MET:HB3	1.87	0.44
2:D:11:GLU:HG3	2:D:12:ASN:HB2	2.00	0.44
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.98	0.43
1:A:108:LEU:HD13	1:A:234:TRP:CD2	2.52	0.43
1:A:114:GLU:HA	1:A:265:SER:O	2.18	0.43
1:C:99:PRO:HB2	1:C:229:ARG:HD3	2.00	0.43
1:C:161:PHE:HB3	1:C:248:ASN:O	2.17	0.43
1:C:172:ARG:HD3	1:C:259:PHE:CE2	2.53	0.43
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.64	0.43
1:C:116:GLY:HA2	1:C:265:SER:HB3	1.99	0.43
1:C:200:LYS:HA	1:C:200:LYS:HD3	1.80	0.43
1:C:180:TRP:NE1	1:C:233:HIS:HB2	2.34	0.43
1:C:71:ILE:CG2	1:C:151:MET:HE3	2.44	0.43
1:C:182:VAL:HG22	1:C:202:ILE:HD12	2.01	0.43
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.84	0.43
1:A:82:PHE:CE2	1:A:117:GLY:HA2	2.53	0.43
1:A:199:ASN:O	1:A:248:ASN:ND2	2.52	0.43
1:A:101:ARG:NH1	1:A:105:GLU:OE2	2.52	0.43
1:C:203:THR:HG23	1:C:246:THR:HB	2.00	0.43
1:C:98:TYR:CD1	1:C:230:ILE:HG13	2.54	0.42
2:D:106:HIS:CE1	2:D:110:LEU:HD23	2.54	0.42
2:D:117:LYS:HB2	2:D:117:LYS:HE3	1.83	0.42
2:B:117:LYS:HB2	2:B:117:LYS:HE3	1.80	0.42
1:C:42:THR:OG1	1:C:314:LEU:O	2.35	0.42
2:B:27:GLN:HA	2:B:31:GLY:O	2.18	0.42
2:B:110:LEU:O	2:B:113:SER:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:PHE:CD1	2:B:170:ARG:HG3	2.55	0.42
1:C:72:GLY:HA3	1:C:149:SER:HB3	2.02	0.42
1:A:83:LYS:HD3	1:A:262:ASN:HB2	2.02	0.42
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.68	0.42
1:C:173:LYS:O	1:C:239:PRO:HG3	2.20	0.42
2:D:67:ASP:CG	2:D:85:ARG:HH22	2.27	0.42
2:D:125:GLN:NE2	2:D:155:ASN:HA	2.32	0.42
1:A:108:LEU:HD22	1:A:234:TRP:CD1	2.55	0.42
1:A:144:VAL:HG12	3:F:1:NAG:H5	2.01	0.42
1:A:146:SER:OG	1:A:147:PHE:N	2.53	0.42
1:A:197:THR:HG22	1:A:198:GLY:N	2.35	0.42
2:B:51:LYS:O	2:B:52:LEU:HB3	2.20	0.42
1:C:67:LEU:HG	1:C:109:ARG:HG2	2.02	0.42
1:C:150:GLU:OE1	1:C:256:ARG:NH1	2.50	0.42
1:A:304:LYS:HE2	1:A:304:LYS:HB3	1.79	0.42
2:B:55:LEU:HD23	2:B:99:LEU:CD2	2.48	0.42
1:C:109:ARG:O	1:C:113:ARG:HG3	2.19	0.42
2:B:106:HIS:CE1	2:B:110:LEU:HD23	2.55	0.41
2:D:61:LYS:C	2:D:61:LYS:HD3	2.44	0.41
2:D:115:MET:HE3	2:D:115:MET:HA	2.01	0.41
1:A:166:GLN:O	1:A:245:PHE:N	2.38	0.41
2:D:52:LEU:N	2:D:55:LEU:HD12	2.33	0.41
1:A:109:ARG:O	1:A:113:ARG:HG3	2.20	0.41
1:C:18:HIS:CE1	1:C:37:VAL:HG11	2.47	0.41
1:C:62:GLY:HA2	1:C:90:ARG:HG3	2.02	0.41
1:A:291:PRO:O	2:B:56:ILE:HD11	2.20	0.41
1:C:161:PHE:HA	1:C:162:PRO:HD3	1.75	0.41
2:B:67:ASP:OD1	2:B:67:ASP:N	2.53	0.41
1:C:197:THR:HG22	1:C:198:GLY:N	2.36	0.41
1:A:169:ARG:HB2	1:A:242:THR:HG22	2.03	0.41
1:A:203:THR:HG23	1:A:246:THR:HB	2.03	0.41
2:B:9:PHE:CZ	2:B:10:ILE:CD1	3.04	0.41
2:B:115:MET:HE3	2:B:115:MET:HA	2.03	0.41
1:C:89:GLU:OE2	1:C:113:ARG:NH2	2.47	0.41
1:C:108:LEU:HD13	1:C:234:TRP:CE3	2.56	0.41
1:C:156:SER:O	1:C:157:SER:OG	2.22	0.41
1:C:82:PHE:CE2	1:C:117:GLY:HA2	2.55	0.41
2:D:28:ASN:ND2	2:D:145:ASP:HA	2.36	0.41
1:A:56:LYS:HE3	1:A:279:GLY:O	2.22	0.40
1:A:73:PRO:HD2	1:A:76:CYS:HB2	2.02	0.40
1:A:110:GLN:HA	1:A:113:ARG:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:HA	1:A:162:PRO:HD3	1.74	0.40
2:B:51:LYS:HD3	2:B:54:ARG:HH12	1.87	0.40
2:B:126:LEU:HD23	2:B:157:TYR:CE2	2.57	0.40
2:B:85:ARG:HH11	2:B:85:ARG:HD2	1.72	0.40
1:C:130:ILE:HG22	1:C:131:ARG:O	2.21	0.40
2:D:158:ASN:CG	4:D:301:NAG:O7	2.63	0.40
1:C:83:LYS:HD3	1:C:262:ASN:HB2	2.04	0.40
1:C:261(A):SER:HB3	1:C:264:LYS:H	1.85	0.40
1:A:66:ILE:HD11	1:A:112:ILE:HG22	2.04	0.40
1:A:201:LEU:HD11	1:A:212:SER:HB2	2.03	0.40
1:C:158:MET:HB2	1:C:159:GLN:OE1	2.21	0.40
1:C:326:LYS:H	2:D:12:ASN:ND2	2.03	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	326/332 (98%)	317 (97%)	7 (2%)	2 (1%)	21	52
1	C	326/332 (98%)	315 (97%)	9 (3%)	2 (1%)	21	52
2	B	167/193 (86%)	159 (95%)	8 (5%)	0	100	100
2	D	167/193 (86%)	160 (96%)	7 (4%)	0	100	100
All	All	986/1050 (94%)	951 (96%)	31 (3%)	4 (0%)	30	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	C	141	ARG
1	A	261(G)	ILE

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Mol	Chain	Res	Type
1	C	261(G)	ILE

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	278/280 (99%)	274 (99%)	4 (1%)	59	76
1	C	278/280 (99%)	272 (98%)	6 (2%)	45	71
2	B	145/163 (89%)	144 (99%)	1 (1%)	76	82
2	D	145/163 (89%)	144 (99%)	1 (1%)	76	82
All	All	846/886 (96%)	834 (99%)	12 (1%)	59	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ARG
1	A	264	LYS
1	A	276	GLU
1	A	276(A)	SER
2	B	61	LYS
1	C	126	ARG
1	C	158	MET
1	C	158(A)	ASN
1	C	158(B)	ASN
1	C	248	ASN
1	C	264	LYS
2	D	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	165	ASN
1	A	166	GLN

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Mol	Chain	Res	Type
2	B	105	GLN
1	C	18	HIS
1	C	75	GLN
2	D	26	HIS
2	D	105	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 ⓘ

4 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	3,1	14,14,15	0.88	2 (14%)	17,19,21	1.32	2 (11%)
3	NAG	E	2	3	14,14,15	0.34	0	17,19,21	0.78	0
3	NAG	F	1	3,1	14,14,15	0.88	2 (14%)	17,19,21	1.32	2 (11%)
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	0.77	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	3,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	NAG	O5-C1	-2.23	1.39	1.43
3	F	1	NAG	O5-C1	-2.23	1.39	1.43
3	E	1	NAG	C2-N2	-2.05	1.42	1.46
3	F	1	NAG	C2-N2	-2.05	1.42	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O5-C5-C6	2.88	113.27	107.66
3	E	1	NAG	O5-C5-C6	2.88	113.26	107.66
3	E	1	NAG	C2-N2-C7	-2.24	119.90	122.90
3	F	1	NAG	C2-N2-C7	-2.23	119.91	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

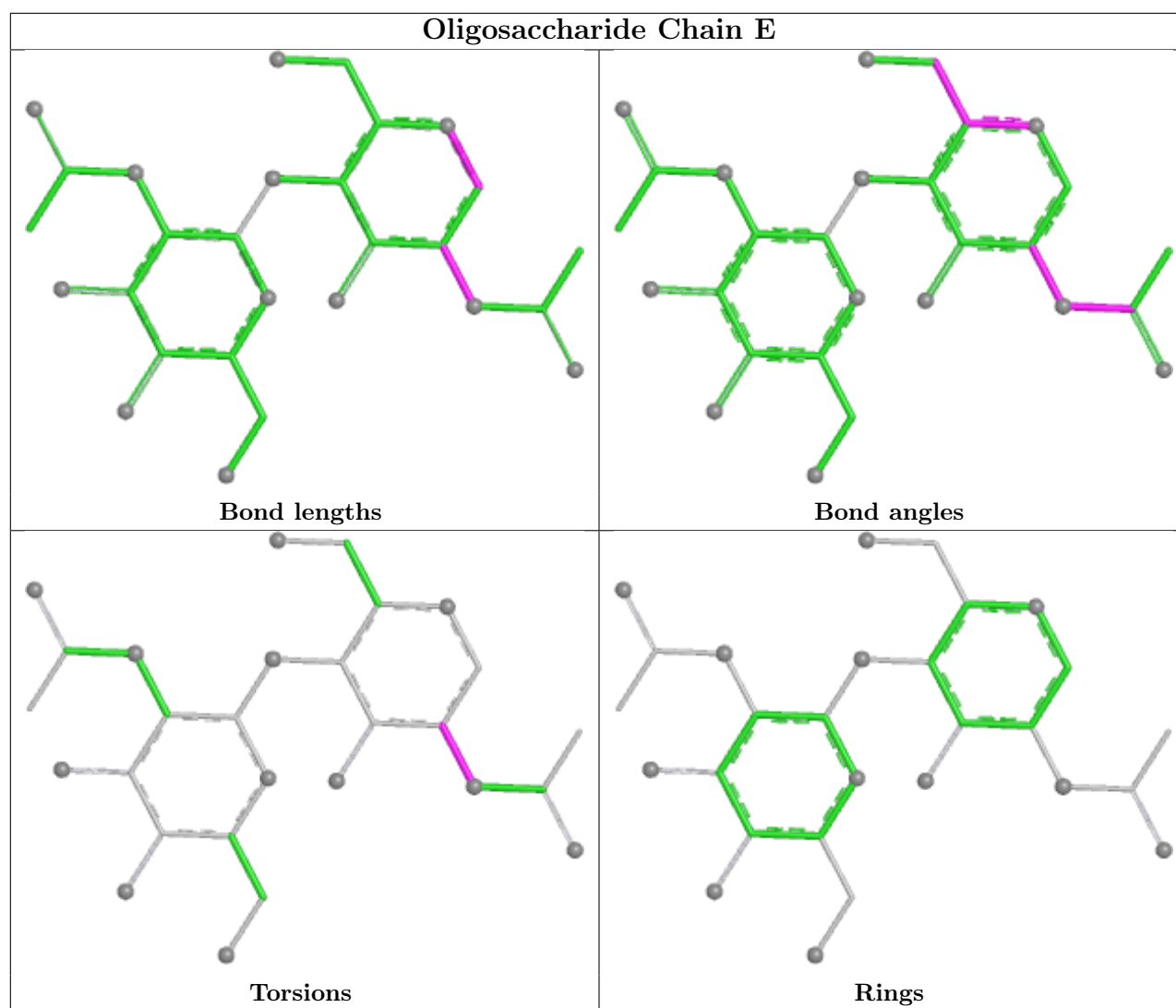
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C1-C2-N2-C7

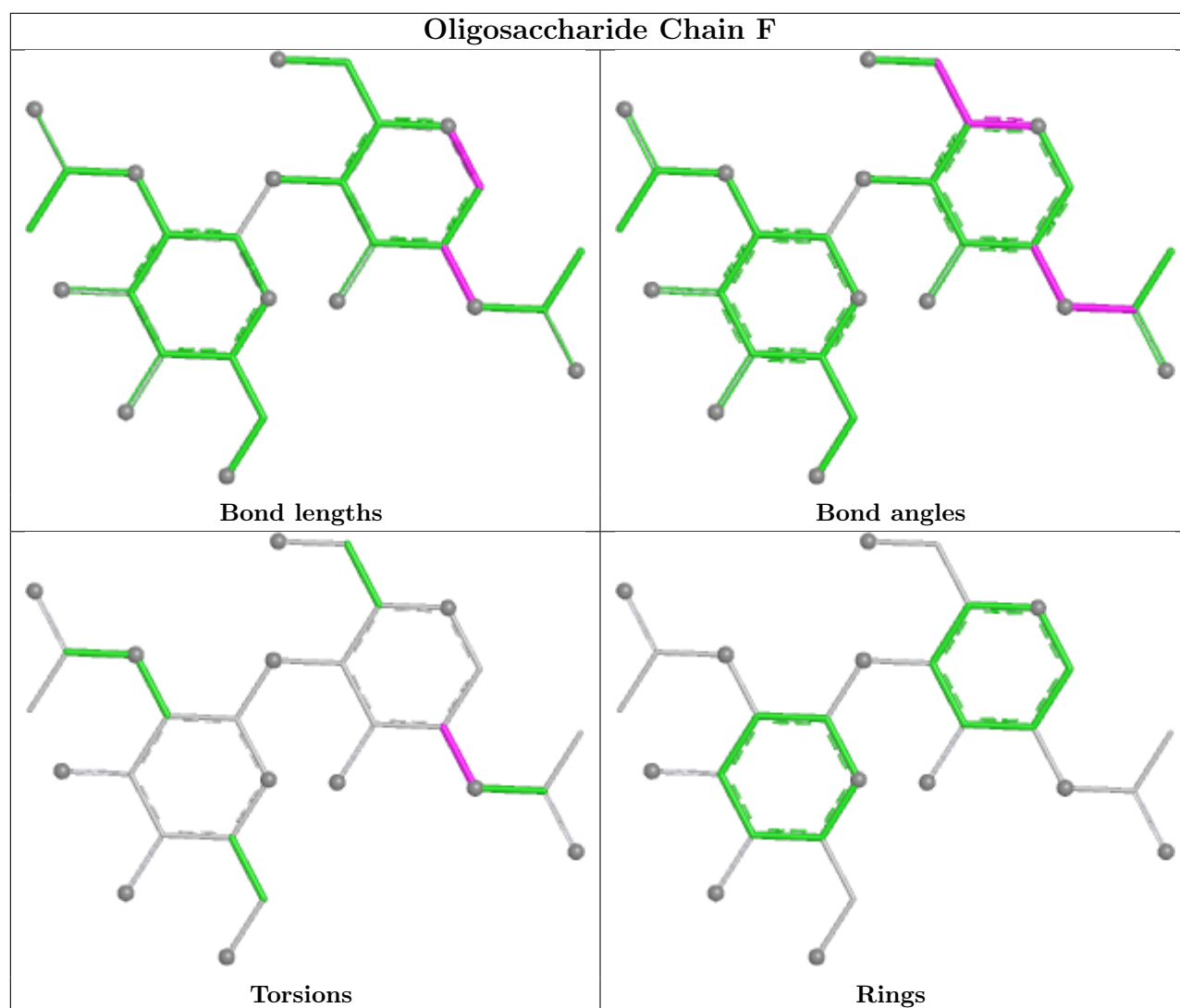
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

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	B	301	2	14,14,15	0.86	1 (7%)	17,19,21	1.79	1 (5%)
4	NAG	D	301	2	14,14,15	0.78	1 (7%)	17,19,21	1.24	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	B	301	2	-	2/6/23/26	0/1/1/1
4	NAG	D	301	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	NAG	O5-C1	-2.39	1.39	1.43
4	D	301	NAG	O5-C1	-2.37	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	C1-C2-N2	5.74	119.48	110.43
4	D	301	NAG	O5-C5-C6	3.44	114.36	107.66

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	C1-C2-N2-C7
4	D	301	NAG	C1-C2-N2-C7
4	D	301	NAG	O7-C7-N2-C2
4	D	301	NAG	C8-C7-N2-C2
4	D	301	NAG	O5-C5-C6-O6
4	B	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	NAG	1	0

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 [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	328/332 (98%)	-1.46	0 100 100	26, 50, 77, 90	0
1	C	328/332 (98%)	-1.43	0 100 100	26, 49, 76, 94	0
2	B	169/193 (87%)	-1.51	0 100 100	24, 38, 70, 89	0
2	D	169/193 (87%)	-1.47	0 100 100	25, 39, 68, 87	0
All	All	994/1050 (94%)	-1.46	0 100 100	24, 44, 76, 94	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

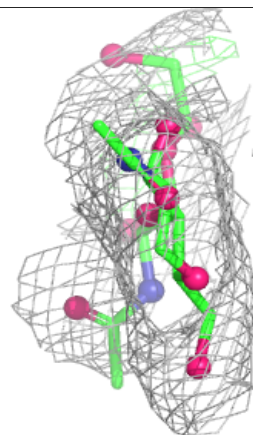
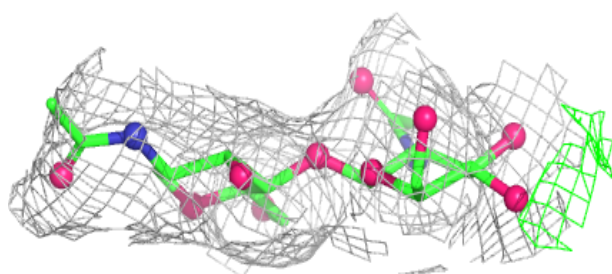
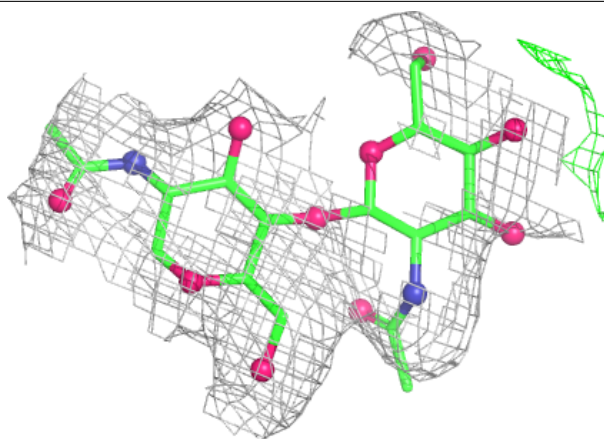
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

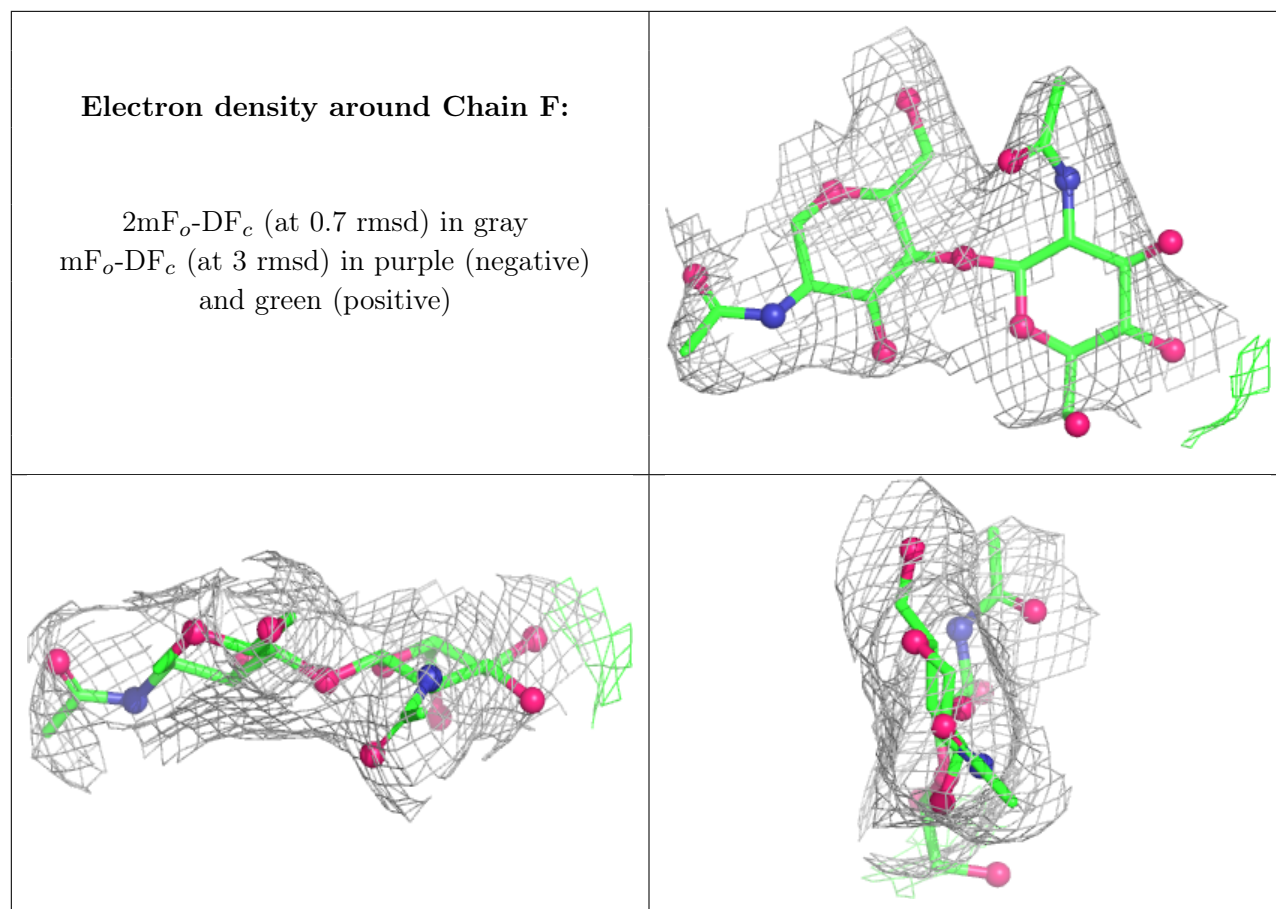
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	1	14/15	0.99	0.03	40,47,54,64	0
3	NAG	E	2	14/15	0.99	0.05	53,64,75,83	0
3	NAG	F	1	14/15	0.99	0.03	43,50,57,64	0
3	NAG	F	2	14/15	0.99	0.04	54,67,80,88	0

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.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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	B	301	14/15	0.98	0.04	57,70,81,84	0
4	NAG	D	301	14/15	0.98	0.05	61,67,76,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.