



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:19 AM UTC

PDB ID : 4K66 / pdb_00004k66
Title : Structure of an airborne transmissible avian influenza H5 hemagglutinin mutant from the influenza virus A/Indonesia/5/2005 complexed with avian receptor analog LSTa
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Qi, J.; Gao, G.F.
Deposited on : 2013-04-15
Resolution : 3.00 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

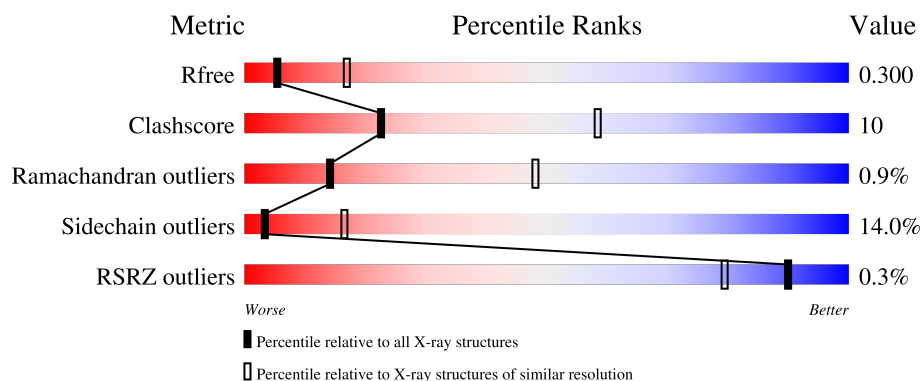
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	321	 66% 28% 5%
1	C	321	 61% 33% 5%
1	E	321	 66% 30% 5%
1	G	321	 67% 30% 5%
2	B	164	 66% 29% 5%

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Mol	Chain	Length	Quality of chain
2	D	164	68%28%
2	F	164	% 62%31%6%
2	H	164	2% 60%34%5%
3	I	2	50%50%
3	J	2	50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15572 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			

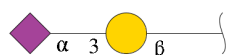
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP A8HWY8
A	107	TYR	HIS	engineered mutation	UNP A8HWY8
A	160	ALA	THR	engineered mutation	UNP A8HWY8
A	226	LEU	GLN	engineered mutation	UNP A8HWY8
A	228	SER	GLY	engineered mutation	UNP A8HWY8
C	4	GLN	-	expression tag	UNP A8HWY8
C	107	TYR	HIS	engineered mutation	UNP A8HWY8
C	160	ALA	THR	engineered mutation	UNP A8HWY8
C	226	LEU	GLN	engineered mutation	UNP A8HWY8
C	228	SER	GLY	engineered mutation	UNP A8HWY8
E	4	GLN	-	expression tag	UNP A8HWY8
E	107	TYR	HIS	engineered mutation	UNP A8HWY8
E	160	ALA	THR	engineered mutation	UNP A8HWY8
E	226	LEU	GLN	engineered mutation	UNP A8HWY8
E	228	SER	GLY	engineered mutation	UNP A8HWY8
G	4	GLN	-	expression tag	UNP A8HWY8
G	107	TYR	HIS	engineered mutation	UNP A8HWY8
G	160	ALA	THR	engineered mutation	UNP A8HWY8
G	226	LEU	GLN	engineered mutation	UNP A8HWY8
G	228	SER	GLY	engineered mutation	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

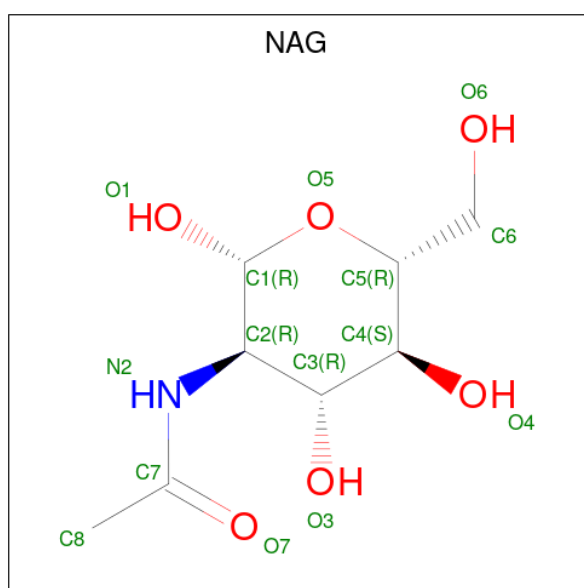
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	D	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	F	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	H	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	J	2	Total	C	N	O	0	0	0
			32	17	1	14			

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

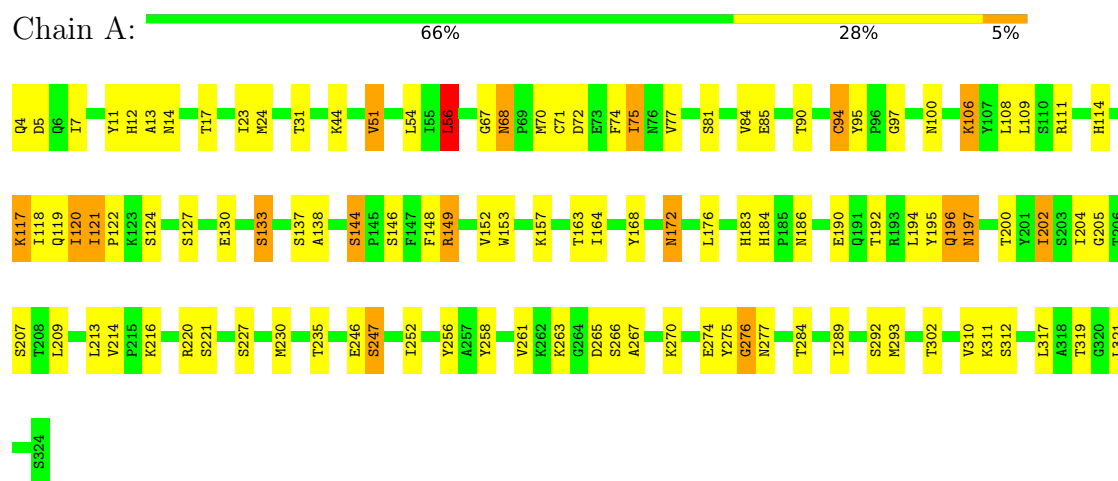


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

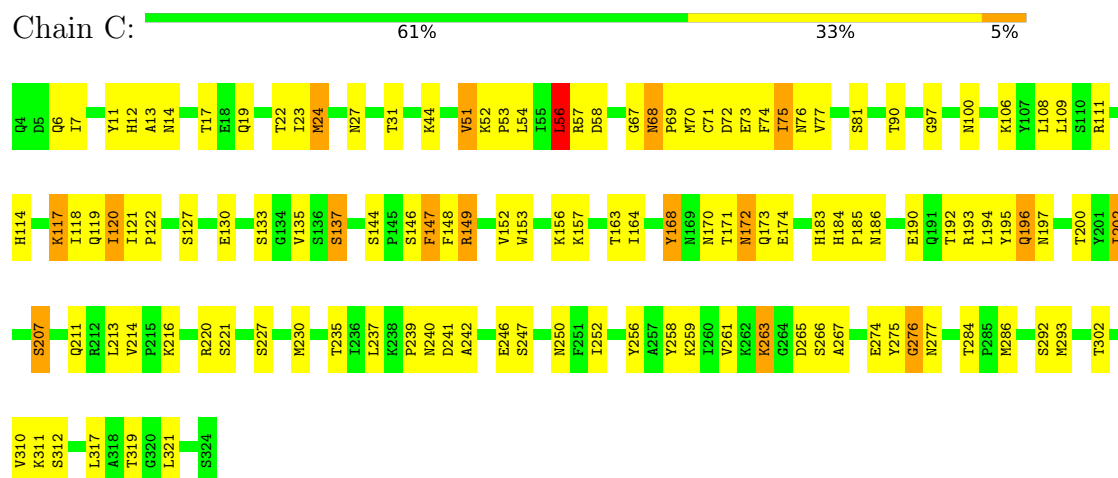
3 Residue-property plots

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

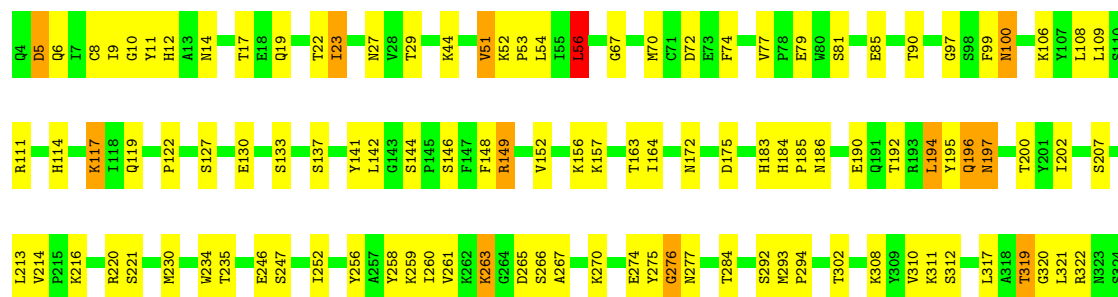


• Molecule 1: Hemagglutinin



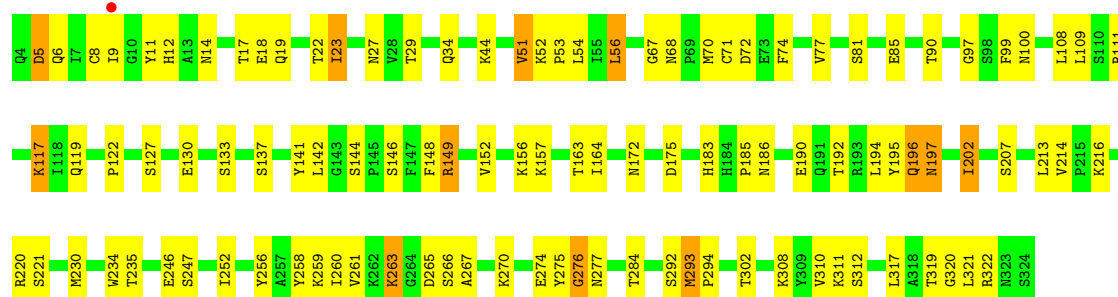
• Molecule 1: Hemagglutinin





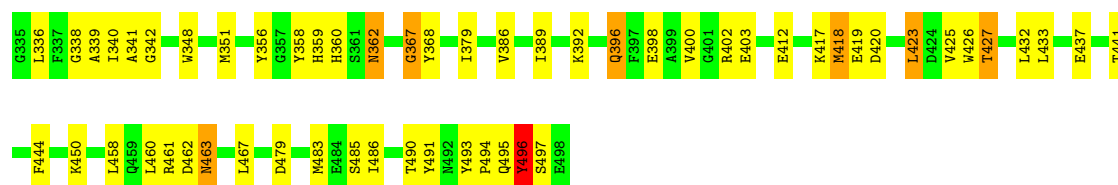
• Molecule 1: Hemagglutinin

Chain G: 67% 30%



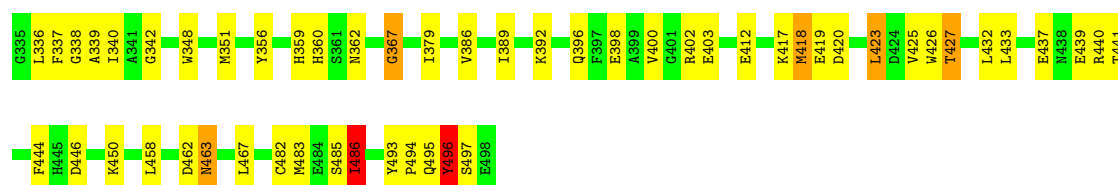
• Molecule 2: Hemagglutinin

Chain B: 66% 29%



• Molecule 2: Hemagglutinin

Chain D: 68% 28%



• Molecule 2: Hemagglutinin

Chain F: 62% 31% 6%

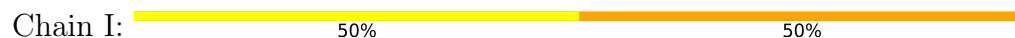




• Molecule 2: Hemagglutinin



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.61Å 70.61Å 490.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 3.00 49.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.01-3.00) 91.7 (49.01-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.219 , 0.262 (Not available) , 0.300	Depositor DCC
R_{free} test set	2545 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.398 for -h,-k,l 0.073 for h,-h-k,-l 0.065 for -k,-h,-l	Xtriage
Reported twinning fraction	0.255 for -h,-k,l	Depositor
Outliers	0 of 50058 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15572	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: GAL, NAG, SIA

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	1.10	4/2604 (0.2%)	1.24	20/3539 (0.6%)
1	C	1.10	3/2604 (0.1%)	1.22	17/3539 (0.5%)
1	E	0.64	0/2604	1.05	10/3539 (0.3%)
1	G	0.63	0/2604	1.01	5/3539 (0.1%)
2	B	0.85	1/1355 (0.1%)	1.09	3/1823 (0.2%)
2	D	0.82	0/1355	1.15	6/1823 (0.3%)
2	F	0.59	0/1355	0.92	2/1823 (0.1%)
2	H	0.61	1/1355 (0.1%)	0.96	3/1823 (0.2%)
All	All	0.84	9/15836 (0.1%)	1.10	66/21448 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	396	GLN	CA-C	7.96	1.56	1.52
1	A	100	ASN	CG-ND2	7.11	1.48	1.33
1	A	100	ASN	CG-OD1	6.96	1.36	1.23
1	A	120	ILE	CA-CB	-6.17	1.47	1.54
1	C	120	ILE	CA-CB	-5.89	1.47	1.54
1	A	94	CYS	C-O	-5.67	1.17	1.24
2	H	362	ASN	N-CA	5.58	1.49	1.46
1	C	76	ASN	CA-C	-5.13	1.46	1.52
1	C	147	PHE	CA-C	-5.10	1.46	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	5	ASP	N-CA-CB	-12.07	92.79	110.17
2	D	440	ARG	NE-CZ-NH2	10.89	129.00	119.20
2	D	440	ARG	NE-CZ-NH1	-10.29	111.22	121.50
1	E	5	ASP	N-CA-C	9.45	123.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6	GLN	N-CA-C	8.82	121.47	108.60
1	E	6	GLN	N-CA-C	8.46	121.00	108.14
2	D	486	ILE	CB-CA-C	-7.67	101.97	112.02
2	D	440	ARG	CD-NE-CZ	7.60	135.04	124.40
2	B	367	GLY	N-CA-C	7.44	121.10	110.46
2	H	362	ASN	N-CA-C	7.31	119.09	108.34
1	C	56	LEU	N-CA-C	-6.98	100.85	110.35
1	C	276	GLY	N-CA-C	-6.71	102.04	112.85
2	H	361	SER	N-CA-C	6.70	119.27	107.61
1	A	100	ASN	N-CA-C	6.66	119.67	110.35
1	A	276	GLY	N-CA-C	-6.59	101.98	112.66
1	C	184	HIS	CA-C-N	6.51	126.89	119.92
1	C	184	HIS	C-N-CA	6.51	126.89	119.92
1	A	184	HIS	CA-C-N	6.49	126.44	120.21
1	A	184	HIS	C-N-CA	6.49	126.44	120.21
1	C	100	ASN	N-CA-C	6.43	119.30	110.24
1	A	56	LEU	N-CA-C	-6.30	101.79	110.35
1	C	68	ASN	CA-C-N	-6.19	113.58	120.45
1	C	68	ASN	C-N-CA	-6.19	113.58	120.45
1	A	14	ASN	N-CA-C	6.06	116.01	108.19
1	A	202	ILE	CB-CA-C	-6.00	103.59	110.73
1	E	276	GLY	N-CA-C	-5.95	103.27	112.85
1	C	14	ASN	N-CA-C	5.91	115.82	108.19
2	H	367	GLY	N-CA-C	5.91	119.76	111.14
1	C	250	ASN	N-CA-C	5.89	119.67	111.90
1	G	276	GLY	N-CA-C	-5.86	103.41	112.85
1	A	121	ILE	CA-C-N	5.83	125.85	119.90
1	A	121	ILE	C-N-CA	5.83	125.85	119.90
1	A	95	TYR	N-CA-C	-5.80	102.47	109.72
2	D	367	GLY	N-CA-C	5.79	118.92	110.63
1	A	204	ILE	CB-CA-C	-5.71	102.36	110.12
1	C	75	ILE	CB-CA-C	-5.55	104.77	112.04
1	C	114	HIS	N-CA-C	5.51	117.02	107.93
1	A	144	SER	CA-C-N	5.48	126.69	119.84
1	A	144	SER	C-N-CA	5.48	126.69	119.84
1	C	200	THR	N-CA-C	5.46	116.93	109.18
1	G	5	ASP	N-CA-C	5.42	117.76	109.95
1	C	202	ILE	CB-CA-C	-5.41	104.29	110.73
1	A	68	ASN	CA-C-N	-5.35	114.18	120.12
1	A	68	ASN	C-N-CA	-5.35	114.18	120.12
1	G	14	ASN	N-CA-C	5.33	115.07	108.19
2	B	336	LEU	N-CA-C	-5.31	105.54	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	336	LEU	N-CA-C	-5.30	105.55	112.23
1	E	184	HIS	CA-C-N	5.30	126.04	120.11
1	E	184	HIS	C-N-CA	5.30	126.04	120.11
1	E	14	ASN	N-CA-C	5.26	114.98	108.19
2	F	367	GLY	N-CA-C	5.25	118.38	110.18
1	C	173	GLN	N-CA-C	-5.23	106.90	113.28
1	A	114	HIS	N-CA-C	5.21	116.53	107.93
1	C	211	GLN	N-CA-C	5.20	118.20	110.14
2	B	486	ILE	N-CA-C	5.18	115.29	110.42
1	C	168	TYR	N-CA-C	5.17	116.45	107.93
1	G	202	ILE	CB-CA-C	-5.10	104.66	110.73
2	F	490	THR	N-CA-C	5.06	117.62	107.41
1	C	58	ASP	N-CA-C	-5.05	106.43	112.59
1	A	289	ILE	N-CA-C	5.05	115.18	108.11
1	A	75	ILE	CB-CA-C	-5.05	105.43	112.04
1	E	100	ASN	N-CA-C	5.04	116.79	110.24
1	A	200	THR	N-CA-C	5.03	116.32	109.18
1	E	56	LEU	N-CA-C	-5.03	102.94	110.23
1	E	200	THR	N-CA-C	5.01	116.29	109.18
1	A	84	VAL	N-CA-C	5.01	115.06	107.80

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	2542	0	2483	48	0
1	C	2542	0	2483	59	0
1	E	2542	0	2484	69	0
1	G	2542	0	2484	62	0
2	B	1328	0	1231	27	0
2	D	1328	0	1231	27	0
2	F	1328	0	1231	48	0
2	H	1328	0	1231	45	1
3	I	32	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	32	0	28	3	0
4	A	14	0	13	0	0
4	C	14	0	13	2	0
All	All	15572	0	14940	319	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 10.

All (319) 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:12:HIS:HB2	2:F:355:TRP:HA	1.36	1.08
1:G:12:HIS:HB2	2:H:355:TRP:HA	1.46	0.97
1:E:9:ILE:HG23	2:F:452:LEU:HD23	1.53	0.90
1:E:12:HIS:N	2:F:355:TRP:O	2.07	0.88
1:G:9:ILE:HG23	2:H:452:LEU:HD23	1.58	0.86
1:E:11:TYR:HA	2:F:356:TYR:HA	1.61	0.80
1:G:12:HIS:N	2:H:355:TRP:O	2.16	0.78
1:E:294:PRO:HG3	2:F:390:ILE:HG12	1.64	0.77
2:H:483:MET:HA	2:H:486:ILE:HD12	1.66	0.77
1:E:294:PRO:HB3	2:F:390:ILE:HG23	1.67	0.75
1:G:294:PRO:HG3	2:H:390:ILE:HG12	1.71	0.73
2:H:359:HIS:CE1	2:H:366:SER:HB3	2.24	0.71
1:C:216:LYS:O	1:C:220:ARG:NH2	2.24	0.71
1:E:308:LYS:HD2	2:F:396:GLN:HB3	1.73	0.69
1:G:11:TYR:HA	2:H:356:TYR:HA	1.73	0.69
1:G:294:PRO:HB3	2:H:390:ILE:HG23	1.76	0.67
1:A:216:LYS:O	1:A:220:ARG:NH2	2.27	0.67
2:D:483:MET:HA	2:D:486:ILE:HG13	1.78	0.66
1:A:311:LYS:H	2:B:427:THR:HG1	1.42	0.66
1:C:311:LYS:HG3	2:D:423:LEU:HD11	1.77	0.66
1:G:216:LYS:O	1:G:220:ARG:NH2	2.29	0.66
2:F:481:GLU:O	2:F:484:GLU:HB2	1.96	0.66
1:G:308:LYS:HD2	2:H:396:GLN:HB3	1.76	0.65
1:A:44:LYS:HD3	1:A:276:GLY:HA3	1.78	0.65
2:D:418:MET:HG3	2:D:419:GLU:N	2.10	0.65
2:H:481:GLU:O	2:H:484:GLU:HB3	1.96	0.65
1:C:311:LYS:H	2:D:427:THR:HG1	1.45	0.64
2:B:418:MET:HG3	2:B:419:GLU:N	2.13	0.64
2:D:389:ILE:HG12	2:D:433:LEU:HD21	1.79	0.64
1:E:216:LYS:O	1:E:220:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:389:ILE:HG12	2:F:433:LEU:HD21	1.80	0.64
1:C:54:LEU:HD22	1:C:77:VAL:HG11	1.80	0.63
1:C:172:ASN:HD22	1:C:172:ASN:N	1.96	0.63
2:B:389:ILE:HG12	2:B:433:LEU:HD21	1.79	0.63
1:E:317:LEU:HD23	2:F:386:VAL:HG22	1.80	0.63
1:G:317:LEU:HD23	2:H:386:VAL:HG22	1.79	0.63
1:C:72:ASP:OD1	1:C:149:ARG:NH1	2.32	0.62
1:C:153:TRP:CH2	3:J:2:SIA:H112	2.34	0.62
2:H:418:MET:HG3	2:H:419:GLU:N	2.13	0.62
1:A:67:GLY:O	1:A:148:PHE:HA	2.00	0.61
1:E:172:ASN:OD1	1:E:259:LYS:HD3	2.00	0.61
1:E:311:LYS:HE3	2:F:423:LEU:HD21	1.82	0.61
2:F:418:MET:HG3	2:F:419:GLU:N	2.14	0.61
2:B:493:TYR:O	2:B:495:GLN:N	2.32	0.61
2:H:493:TYR:O	2:H:495:GLN:N	2.33	0.61
2:F:479:ASP:OD1	2:F:479:ASP:N	2.34	0.60
2:F:493:TYR:O	2:F:495:GLN:N	2.34	0.60
1:E:44:LYS:HD3	1:E:276:GLY:HA3	1.81	0.60
2:D:493:TYR:O	2:D:495:GLN:N	2.34	0.60
1:G:311:LYS:HE3	2:H:423:LEU:HD21	1.84	0.60
1:C:311:LYS:HE3	2:D:423:LEU:HD21	1.83	0.60
1:G:44:LYS:HD3	1:G:276:GLY:HA3	1.81	0.59
1:A:54:LEU:HD22	1:A:77:VAL:HG11	1.85	0.59
1:E:17:THR:HA	1:E:29:THR:HG23	1.84	0.59
1:G:54:LEU:HD22	1:G:77:VAL:HG11	1.85	0.59
1:G:172:ASN:OD1	1:G:259:LYS:HD3	2.03	0.58
2:H:389:ILE:HG12	2:H:433:LEU:HD21	1.84	0.58
1:C:67:GLY:O	1:C:148:PHE:HA	2.03	0.58
1:G:17:THR:HA	1:G:29:THR:HG23	1.85	0.58
1:C:44:LYS:HD3	1:C:276:GLY:HA3	1.84	0.58
2:H:462:ASP:OD1	2:H:493:TYR:OH	2.21	0.58
1:A:311:LYS:HG3	2:B:423:LEU:HD11	1.86	0.57
1:C:172:ASN:OD1	1:C:259:LYS:HD3	2.04	0.57
1:E:308:LYS:HZ2	2:F:396:GLN:H	1.50	0.57
1:A:72:ASP:OD1	1:A:149:ARG:NH1	2.37	0.57
1:E:266:SER:OG	1:E:267:ALA:N	2.37	0.57
1:C:186:ASN:HB3	1:C:190:GLU:OE1	2.05	0.57
2:F:462:ASP:OD1	2:F:493:TYR:OH	2.22	0.57
1:E:72:ASP:OD1	1:E:149:ARG:NH1	2.37	0.57
1:A:119:GLN:NE2	1:A:122:PRO:HA	2.20	0.56
1:A:311:LYS:HE3	2:B:423:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:SER:OG	2:B:491:TYR:HA	2.05	0.56
1:E:54:LEU:HD22	1:E:77:VAL:HG11	1.86	0.56
2:F:482:CYS:C	2:F:484:GLU:H	2.14	0.56
2:B:462:ASP:OD1	2:B:493:TYR:OH	2.24	0.56
1:C:11:TYR:CZ	2:D:340:ILE:HG23	2.41	0.55
2:D:359:HIS:HA	2:D:367:GLY:O	2.07	0.55
1:G:186:ASN:HB3	1:G:190:GLU:OE1	2.07	0.55
1:E:10:GLY:O	2:F:357:GLY:N	2.35	0.55
1:G:11:TYR:CZ	2:H:340:ILE:HG23	2.42	0.55
1:G:72:ASP:OD1	1:G:149:ARG:NH1	2.40	0.55
1:G:130:GLU:HG2	1:G:157:LYS:HB2	1.90	0.54
2:H:359:HIS:HE1	2:H:366:SER:HB3	1.73	0.54
1:C:130:GLU:HG2	1:C:157:LYS:HB2	1.89	0.54
2:D:462:ASP:OD1	2:D:493:TYR:OH	2.25	0.54
1:A:11:TYR:CZ	2:B:340:ILE:HG23	2.43	0.54
1:C:164:ILE:O	1:C:246:GLU:HA	2.08	0.54
1:E:141:TYR:CE2	1:E:142:LEU:HD12	2.42	0.54
2:D:496:TYR:CG	2:D:497:SER:N	2.75	0.54
1:E:321:LEU:HB3	2:F:445:HIS:CG	2.43	0.54
1:C:266:SER:OG	1:C:267:ALA:N	2.41	0.53
1:A:7:ILE:HD12	2:B:483:MET:SD	2.49	0.53
1:A:186:ASN:HB3	1:A:190:GLU:OE1	2.09	0.53
1:E:186:ASN:HB3	1:E:190:GLU:OE1	2.08	0.53
1:E:311:LYS:HG3	2:F:423:LEU:HD11	1.90	0.53
1:E:119:GLN:HB2	1:E:256:TYR:CE1	2.44	0.52
1:A:56:LEU:HA	1:A:74:PHE:CZ	2.44	0.52
2:B:359:HIS:HA	2:B:367:GLY:O	2.08	0.52
1:E:51:VAL:HG22	1:E:81:SER:HB3	1.91	0.52
1:G:311:LYS:HG3	2:H:423:LEU:HD11	1.91	0.52
1:G:119:GLN:HB2	1:G:256:TYR:CE1	2.45	0.52
1:G:266:SER:OG	1:G:267:ALA:N	2.40	0.52
1:E:130:GLU:HG2	1:E:157:LYS:HB2	1.92	0.51
1:G:119:GLN:NE2	1:G:122:PRO:HA	2.26	0.51
2:F:348:TRP:HE3	2:F:351:MET:HE2	1.75	0.51
1:G:141:TYR:CE2	1:G:142:LEU:HD12	2.44	0.51
1:A:51:VAL:HG22	1:A:81:SER:HB3	1.93	0.51
1:E:119:GLN:NE2	1:E:122:PRO:HA	2.26	0.51
1:E:320:GLY:HA2	2:F:355:TRP:CZ2	2.46	0.51
2:F:496:TYR:CG	2:F:497:SER:N	2.76	0.51
1:E:17:THR:HG22	1:E:29:THR:HG21	1.92	0.51
2:H:348:TRP:HE3	2:H:351:MET:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:GLY:O	1:E:148:PHE:HA	2.10	0.51
1:C:119:GLN:HB2	1:C:256:TYR:CE1	2.46	0.50
1:C:242:ALA:H	4:C:601:NAG:H82	1.75	0.50
1:A:164:ILE:O	1:A:246:GLU:HA	2.12	0.50
1:C:171:THR:C	1:C:172:ASN:HD22	2.20	0.50
1:A:11:TYR:O	2:B:348:TRP:N	2.25	0.50
1:E:9:ILE:HD13	2:F:453:TYR:HA	1.94	0.50
1:G:51:VAL:HG22	1:G:81:SER:HB3	1.94	0.50
1:G:97:GLY:HA3	1:G:230:MET:O	2.12	0.50
2:B:496:TYR:CG	2:B:497:SER:N	2.77	0.49
2:D:339:ALA:HB2	2:D:450:LYS:HB2	1.94	0.49
1:E:56:LEU:HA	1:E:74:PHE:CZ	2.47	0.49
1:E:172:ASN:N	1:E:172:ASN:HD22	2.09	0.49
1:G:317:LEU:HD13	2:H:434:VAL:HG22	1.92	0.49
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.52	0.49
1:C:56:LEU:HA	1:C:74:PHE:CZ	2.47	0.49
1:G:9:ILE:HD13	2:H:453:TYR:HA	1.95	0.49
1:E:317:LEU:HD13	2:F:434:VAL:HG22	1.95	0.49
1:A:172:ASN:N	1:A:172:ASN:HD22	2.09	0.49
2:D:482:CYS:O	2:D:485:SER:OG	2.18	0.49
2:B:417:LYS:HB3	2:B:417:LYS:HE3	1.60	0.49
2:H:486:ILE:HA	2:H:491:TYR:HB2	1.94	0.49
1:E:97:GLY:HA3	1:E:230:MET:O	2.13	0.49
1:A:119:GLN:HB2	1:A:256:TYR:CE1	2.47	0.48
1:A:130:GLU:HG2	1:A:157:LYS:HB2	1.95	0.48
1:A:274:GLU:HG3	1:A:275:TYR:H	1.78	0.48
1:G:274:GLU:HG3	1:G:275:TYR:H	1.79	0.48
2:H:496:TYR:CG	2:H:497:SER:N	2.76	0.48
1:G:308:LYS:HZ2	2:H:396:GLN:H	1.60	0.48
1:E:8:CYS:HB3	2:F:348:TRP:HH2	1.79	0.48
2:F:359:HIS:CE1	2:F:366:SER:HB3	2.48	0.48
1:G:67:GLY:O	1:G:148:PHE:HA	2.13	0.48
2:H:463:ASN:N	2:H:463:ASN:OD1	2.47	0.48
2:B:339:ALA:HB2	2:B:450:LYS:HB2	1.96	0.48
1:C:52:LYS:HG2	1:C:53:PRO:HD2	1.96	0.48
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.54	0.48
1:A:97:GLY:HA3	1:A:230:MET:O	2.12	0.48
1:G:172:ASN:N	1:G:172:ASN:HD22	2.11	0.48
1:A:317:LEU:HD23	2:B:386:VAL:HG22	1.96	0.47
1:E:12:HIS:HB2	2:F:355:TRP:CA	2.24	0.47
1:G:192:THR:HG22	1:G:196:GLN:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLY:O	2:B:342:GLY:HA3	2.14	0.47
2:H:339:ALA:HB2	2:H:450:LYS:HB2	1.96	0.47
1:C:106:LYS:NZ	2:D:403:GLU:OE2	2.41	0.47
1:E:308:LYS:HE3	2:F:394:ASN:O	2.14	0.47
1:C:7:ILE:HD12	2:D:483:MET:SD	2.54	0.47
1:C:195:TYR:O	1:C:197:ASN:N	2.47	0.47
1:E:9:ILE:CG2	2:F:452:LEU:HD23	2.37	0.47
1:E:11:TYR:CZ	2:F:340:ILE:HG23	2.50	0.47
2:F:339:ALA:HB2	2:F:450:LYS:HB2	1.97	0.47
1:G:34:GLN:OE1	2:H:386:VAL:HG21	2.15	0.47
1:A:202:ILE:HA	1:A:247:SER:HB2	1.96	0.47
2:B:362:ASN:ND2	2:B:479:ASP:HA	2.29	0.47
1:C:51:VAL:HG22	1:C:81:SER:HB3	1.95	0.47
1:C:317:LEU:HD23	2:D:386:VAL:HG22	1.96	0.47
1:G:196:GLN:HE21	1:G:196:GLN:HA	1.79	0.47
2:H:359:HIS:HA	2:H:367:GLY:O	2.14	0.47
1:G:56:LEU:HA	1:G:74:PHE:CZ	2.50	0.47
1:G:321:LEU:HB3	2:H:445:HIS:CG	2.50	0.47
1:C:119:GLN:NE2	1:C:122:PRO:HA	2.30	0.46
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.96	0.46
1:C:69:PRO:HG3	1:C:147:PHE:O	2.14	0.46
1:E:195:TYR:O	1:E:197:ASN:N	2.48	0.46
2:H:482:CYS:C	2:H:484:GLU:H	2.21	0.46
1:C:137:SER:OG	3:J:2:SIA:O1A	2.32	0.46
2:F:463:ASN:OD1	2:F:463:ASN:N	2.49	0.46
1:E:12:HIS:HB3	2:F:355:TRP:HD1	1.81	0.46
1:A:72:ASP:OD2	1:A:149:ARG:HD2	2.15	0.46
1:C:97:GLY:HA3	1:C:230:MET:O	2.15	0.46
2:F:359:HIS:HA	2:F:367:GLY:O	2.15	0.46
2:D:348:TRP:HE3	2:D:351:MET:HE2	1.81	0.46
1:A:133:SER:O	3:I:2:SIA:H113	2.15	0.46
1:A:168:TYR:CD2	1:A:168:TYR:C	2.90	0.46
1:E:99:PHE:HE2	1:E:234:TRP:CD1	2.34	0.46
2:B:360:HIS:HB2	2:B:483:MET:HE3	1.98	0.45
1:E:52:LYS:HG2	1:E:53:PRO:HD2	1.97	0.45
1:A:44:LYS:HD3	1:A:276:GLY:CA	2.45	0.45
2:B:348:TRP:HE3	2:B:351:MET:HE2	1.81	0.45
2:B:396:GLN:HG3	2:B:426:TRP:CD2	2.52	0.45
2:D:337:PHE:HB2	2:D:446:ASP:OD2	2.16	0.45
1:C:274:GLU:HG3	1:C:275:TYR:H	1.81	0.45
2:D:463:ASN:OD1	2:D:463:ASN:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ILE:HA	2:H:435:LEU:HD13	1.98	0.45
1:C:183:HIS:O	1:C:185:PRO:HD3	2.16	0.45
2:D:360:HIS:HB2	2:D:483:MET:HE3	1.97	0.45
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.98	0.45
2:H:360:HIS:HB2	2:H:483:MET:HE3	1.98	0.45
1:A:266:SER:OG	1:A:267:ALA:N	2.43	0.45
1:C:220:ARG:HD2	1:C:227:SER:O	2.17	0.45
2:D:441:THR:O	2:D:444:PHE:HB3	2.16	0.45
1:G:263:LYS:H	1:G:263:LYS:HG2	1.44	0.45
1:A:153:TRP:CH2	3:I:2:SIA:H112	2.52	0.45
2:B:463:ASN:OD1	2:B:463:ASN:N	2.49	0.45
1:A:195:TYR:O	1:A:197:ASN:N	2.50	0.45
1:E:164:ILE:O	1:E:246:GLU:HA	2.17	0.45
1:E:319:THR:O	2:F:382:VAL:HG11	2.17	0.45
1:G:19:GLN:HB3	1:G:27:ASN:C	2.42	0.45
1:E:321:LEU:HB3	2:F:445:HIS:ND1	2.32	0.44
1:A:106:LYS:NZ	2:B:403:GLU:OE2	2.43	0.44
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.99	0.44
1:E:192:THR:HG22	1:E:196:GLN:O	2.16	0.44
1:E:274:GLU:HG3	1:E:275:TYR:H	1.82	0.44
1:C:44:LYS:HD3	1:C:276:GLY:CA	2.47	0.44
1:C:75:ILE:HD13	1:C:75:ILE:HG21	1.65	0.44
1:E:119:GLN:HE21	1:E:122:PRO:HA	1.82	0.44
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.98	0.44
1:A:117:LYS:HD3	1:A:258:TYR:CE1	2.52	0.44
1:A:220:ARG:HD2	1:A:227:SER:O	2.17	0.44
1:C:202:ILE:HA	1:C:247:SER:HB2	2.00	0.44
1:E:79:GLU:HB2	1:E:114:HIS:CD2	2.52	0.44
2:F:360:HIS:HB2	2:F:483:MET:HE3	1.99	0.44
2:F:488:ASN:HB2	2:F:489:GLY:H	1.62	0.44
1:G:195:TYR:O	1:G:197:ASN:N	2.50	0.44
2:F:482:CYS:C	2:F:484:GLU:N	2.76	0.44
1:G:52:LYS:HG2	1:G:53:PRO:HD2	1.98	0.44
2:H:398:GLU:H	2:H:398:GLU:HG2	1.64	0.44
2:H:441:THR:O	2:H:444:PHE:HB3	2.17	0.44
1:A:119:GLN:HE21	1:A:122:PRO:HA	1.81	0.44
1:E:23:ILE:HA	2:F:435:LEU:HD13	2.00	0.44
2:D:396:GLN:HG3	2:D:426:TRP:CD2	2.52	0.44
1:E:19:GLN:HB3	1:E:27:ASN:C	2.43	0.44
2:B:441:THR:O	2:B:444:PHE:HB3	2.17	0.44
1:E:11:TYR:C	2:F:355:TRP:O	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLU:O	1:E:270:LYS:HA	2.18	0.43
1:E:263:LYS:H	1:E:263:LYS:HG2	1.43	0.43
2:F:441:THR:O	2:F:444:PHE:HB3	2.17	0.43
1:C:174:GLU:OE1	1:C:259:LYS:HD2	2.18	0.43
1:E:44:LYS:HD3	1:E:276:GLY:CA	2.48	0.43
1:G:183:HIS:O	1:G:185:PRO:HD3	2.19	0.43
1:G:8:CYS:HB3	2:H:348:TRP:HH2	1.84	0.43
1:A:4:GLN:HG2	1:A:5:ASP:H	1.84	0.43
1:A:205:GLY:HA2	1:A:209:LEU:O	2.19	0.43
1:C:192:THR:HG22	1:C:196:GLN:O	2.18	0.43
2:D:423:LEU:O	2:D:423:LEU:HD12	2.18	0.43
1:G:22:THR:C	2:H:435:LEU:HD22	2.43	0.43
1:G:119:GLN:HE21	1:G:122:PRO:HA	1.82	0.43
2:B:460:LEU:O	2:B:461:ARG:C	2.62	0.43
2:D:417:LYS:HB3	2:D:417:LYS:HE3	1.61	0.43
1:E:196:GLN:HA	1:E:196:GLN:HE21	1.83	0.43
1:G:99:PHE:HE2	1:G:234:TRP:CD1	2.37	0.43
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.78	0.43
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.83	0.43
1:C:170:ASN:HB2	1:C:237:LEU:HD13	2.01	0.43
1:C:207:SER:HG	1:C:241:ASP:CG	2.27	0.43
1:C:242:ALA:N	4:C:601:NAG:H82	2.33	0.43
1:G:44:LYS:HD3	1:G:276:GLY:CA	2.49	0.43
2:H:362:ASN:ND2	2:H:479:ASP:HA	2.34	0.43
2:F:485:SER:O	2:F:491:TYR:N	2.52	0.43
1:C:22:THR:HB	2:D:439:GLU:HB2	2.00	0.42
1:G:164:ILE:O	1:G:246:GLU:HA	2.19	0.42
1:A:12:HIS:HD2	1:A:13:ALA:O	2.02	0.42
1:E:72:ASP:OD2	1:E:149:ARG:HD2	2.19	0.42
2:F:396:GLN:HG3	2:F:426:TRP:CD2	2.54	0.42
1:A:120:ILE:C	1:A:121:ILE:HG13	2.44	0.42
2:B:402:ARG:HH11	2:B:402:ARG:HD2	1.69	0.42
1:C:24:MET:HE3	1:C:24:MET:HB2	1.89	0.42
1:A:85:GLU:O	1:A:270:LYS:HA	2.20	0.42
1:C:72:ASP:OD2	1:C:149:ARG:HD2	2.20	0.42
2:H:362:ASN:HB2	2:H:363:GLU:H	1.57	0.42
2:F:479:ASP:HB2	2:F:480:ASN:H	1.72	0.42
1:C:57:ARG:HD2	1:C:73:GLU:OE1	2.19	0.42
1:G:202:ILE:HG23	1:G:247:SER:HB2	2.01	0.42
2:D:338:GLY:O	2:D:342:GLY:HA3	2.20	0.42
1:E:17:THR:HA	1:E:29:THR:CG2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:MET:HG3	1:G:294:PRO:HD2	2.02	0.42
1:C:120:ILE:C	1:C:121:ILE:HG13	2.45	0.42
1:E:311:LYS:CG	2:F:423:LEU:HD11	2.50	0.42
1:G:12:HIS:HB3	2:H:355:TRP:HD1	1.84	0.42
1:G:321:LEU:HD12	1:G:322:ARG:O	2.19	0.42
1:C:19:GLN:HB3	1:C:27:ASN:C	2.45	0.41
2:H:396:GLN:HG3	2:H:426:TRP:CD2	2.55	0.41
1:C:168:TYR:CD2	1:C:168:TYR:C	2.97	0.41
1:E:22:THR:C	2:F:435:LEU:HD22	2.44	0.41
1:A:183:HIS:HB2	1:A:252:ILE:HD11	2.03	0.41
2:H:482:CYS:O	2:H:486:ILE:HG13	2.21	0.41
1:E:117:LYS:HD3	1:E:258:TYR:CE1	2.55	0.41
1:C:156:LYS:HE2	1:C:193:ARG:O	2.20	0.41
1:C:263:LYS:H	1:C:263:LYS:HG2	1.48	0.41
1:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.41
1:G:202:ILE:HA	1:G:247:SER:HB2	2.02	0.41
1:A:31:THR:HG23	1:A:321:LEU:O	2.20	0.41
1:C:117:LYS:HD3	1:C:258:TYR:CE1	2.55	0.41
1:C:153:TRP:CZ3	3:J:2:SIA:H112	2.54	0.41
1:G:85:GLU:O	1:G:270:LYS:HA	2.20	0.41
1:G:156:LYS:HD2	1:G:196:GLN:HG2	2.02	0.41
1:A:75:ILE:HG21	1:A:75:ILE:HD13	1.64	0.41
2:B:358:TYR:O	2:B:368:TYR:HA	2.21	0.41
1:C:183:HIS:CD2	1:C:230:MET:HE2	2.56	0.41
1:E:175:ASP:HB2	1:E:260:ILE:HD12	2.02	0.41
1:E:194:LEU:HB3	1:E:195:TYR:CE1	2.56	0.41
1:E:202:ILE:HA	1:E:247:SER:HB2	2.03	0.41
1:G:68:ASN:HB3	1:G:71:CYS:SG	2.61	0.41
1:G:175:ASP:HB2	1:G:260:ILE:HD12	2.03	0.41
1:A:94:CYS:HB2	1:A:138:ALA:O	2.21	0.41
1:A:192:THR:HG22	1:A:196:GLN:O	2.21	0.41
1:C:239:PRO:O	1:C:240:ASN:HB2	2.21	0.41
1:E:321:LEU:HD12	1:E:322:ARG:O	2.20	0.40
1:G:117:LYS:HD3	1:G:258:TYR:CE1	2.55	0.40
2:H:338:GLY:O	2:H:342:GLY:HA3	2.21	0.40
1:G:17:THR:HA	1:G:29:THR:CG2	2.48	0.40
1:G:308:LYS:HE3	2:H:394:ASN:O	2.21	0.40
1:G:320:GLY:HA2	2:H:355:TRP:CZ2	2.56	0.40
1:C:12:HIS:HD2	1:C:13:ALA:C	2.30	0.40
1:A:274:GLU:HG3	1:A:275:TYR:N	2.36	0.40
1:C:31:THR:HG23	1:C:321:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:ARG:HH11	2:D:402:ARG:HD2	1.71	0.40
1:E:183:HIS:HB2	1:E:252:ILE:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:408:GLU:OE2	2:H:410:ARG:NH2[2_665]	2.15	0.05

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	319/321 (99%)	294 (92%)	24 (8%)	1 (0%)	36	70
1	C	319/321 (99%)	296 (93%)	22 (7%)	1 (0%)	36	70
1	E	319/321 (99%)	293 (92%)	25 (8%)	1 (0%)	36	70
1	G	319/321 (99%)	294 (92%)	23 (7%)	2 (1%)	21	56
2	B	162/164 (99%)	142 (88%)	17 (10%)	3 (2%)	6	30
2	D	162/164 (99%)	140 (86%)	20 (12%)	2 (1%)	10	40
2	F	162/164 (99%)	134 (83%)	24 (15%)	4 (2%)	4	23
2	H	162/164 (99%)	137 (85%)	22 (14%)	3 (2%)	6	30
All	All	1924/1940 (99%)	1730 (90%)	177 (9%)	17 (1%)	14	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	494	PRO
2	B	496	TYR

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Mol	Chain	Res	Type
1	C	196	GLN
2	D	494	PRO
2	D	496	TYR
1	E	196	GLN
2	F	494	PRO
2	F	496	TYR
1	G	196	GLN
2	H	494	PRO
2	H	496	TYR
2	F	483	MET
2	B	341	ALA
2	F	461	ARG
2	H	461	ARG
1	G	18	GLU

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	288/288 (100%)	246 (85%)	42 (15%)	3	15
1	C	288/288 (100%)	247 (86%)	41 (14%)	3	16
1	E	288/288 (100%)	250 (87%)	38 (13%)	4	18
1	G	288/288 (100%)	251 (87%)	37 (13%)	4	19
2	B	140/140 (100%)	121 (86%)	19 (14%)	3	17
2	D	140/140 (100%)	121 (86%)	19 (14%)	3	17
2	F	140/140 (100%)	118 (84%)	22 (16%)	2	13
2	H	140/140 (100%)	118 (84%)	22 (16%)	2	13
All	All	1712/1712 (100%)	1472 (86%)	240 (14%)	3	16

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR

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Mol	Chain	Res	Type
1	A	23	ILE
1	A	24	MET
1	A	51	VAL
1	A	56	LEU
1	A	70	MET
1	A	90	THR
1	A	106	LYS
1	A	108	LEU
1	A	109	LEU
1	A	111	ARG
1	A	117	LYS
1	A	118	ILE
1	A	124	SER
1	A	127	SER
1	A	133	SER
1	A	137	SER
1	A	144	SER
1	A	146	SER
1	A	149	ARG
1	A	152	VAL
1	A	163	THR
1	A	172	ASN
1	A	194	LEU
1	A	197	ASN
1	A	207	SER
1	A	213	LEU
1	A	214	VAL
1	A	221	SER
1	A	235	THR
1	A	247	SER
1	A	261	VAL
1	A	263	LYS
1	A	265	ASP
1	A	277	ASN
1	A	284	THR
1	A	292	SER
1	A	293	MET
1	A	302	THR
1	A	310	VAL
1	A	312	SER
1	A	319	THR
2	B	356	TYR

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Mol	Chain	Res	Type
2	B	362	ASN
2	B	379	ILE
2	B	392	LYS
2	B	398	GLU
2	B	400	VAL
2	B	412	GLU
2	B	418	MET
2	B	420	ASP
2	B	423	LEU
2	B	425	VAL
2	B	427	THR
2	B	432	LEU
2	B	437	GLU
2	B	458	LEU
2	B	463	ASN
2	B	467	LEU
2	B	490	THR
2	B	496	TYR
1	C	6	GLN
1	C	17	THR
1	C	23	ILE
1	C	24	MET
1	C	51	VAL
1	C	56	LEU
1	C	70	MET
1	C	90	THR
1	C	108	LEU
1	C	109	LEU
1	C	111	ARG
1	C	117	LYS
1	C	118	ILE
1	C	127	SER
1	C	133	SER
1	C	135	VAL
1	C	137	SER
1	C	144	SER
1	C	146	SER
1	C	149	ARG
1	C	152	VAL
1	C	163	THR
1	C	172	ASN
1	C	194	LEU

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Mol	Chain	Res	Type
1	C	207	SER
1	C	213	LEU
1	C	214	VAL
1	C	221	SER
1	C	235	THR
1	C	261	VAL
1	C	263	LYS
1	C	265	ASP
1	C	277	ASN
1	C	284	THR
1	C	286	MET
1	C	292	SER
1	C	293	MET
1	C	302	THR
1	C	310	VAL
1	C	312	SER
1	C	319	THR
2	D	356	TYR
2	D	362	ASN
2	D	379	ILE
2	D	392	LYS
2	D	398	GLU
2	D	400	VAL
2	D	412	GLU
2	D	418	MET
2	D	420	ASP
2	D	423	LEU
2	D	425	VAL
2	D	427	THR
2	D	432	LEU
2	D	437	GLU
2	D	458	LEU
2	D	463	ASN
2	D	467	LEU
2	D	486	ILE
2	D	496	TYR
1	E	5	ASP
1	E	23	ILE
1	E	51	VAL
1	E	56	LEU
1	E	70	MET
1	E	90	THR

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Mol	Chain	Res	Type
1	E	100	ASN
1	E	106	LYS
1	E	108	LEU
1	E	109	LEU
1	E	111	ARG
1	E	117	LYS
1	E	127	SER
1	E	133	SER
1	E	137	SER
1	E	144	SER
1	E	146	SER
1	E	149	ARG
1	E	152	VAL
1	E	163	THR
1	E	194	LEU
1	E	197	ASN
1	E	207	SER
1	E	213	LEU
1	E	214	VAL
1	E	221	SER
1	E	235	THR
1	E	261	VAL
1	E	263	LYS
1	E	265	ASP
1	E	277	ASN
1	E	284	THR
1	E	292	SER
1	E	293	MET
1	E	302	THR
1	E	310	VAL
1	E	312	SER
1	E	319	THR
2	F	336	LEU
2	F	356	TYR
2	F	362	ASN
2	F	363	GLU
2	F	392	LYS
2	F	398	GLU
2	F	400	VAL
2	F	412	GLU
2	F	418	MET
2	F	423	LEU

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Mol	Chain	Res	Type
2	F	425	VAL
2	F	427	THR
2	F	432	LEU
2	F	437	GLU
2	F	458	LEU
2	F	463	ASN
2	F	467	LEU
2	F	479	ASP
2	F	488	ASN
2	F	490	THR
2	F	494	PRO
2	F	496	TYR
1	G	5	ASP
1	G	23	ILE
1	G	51	VAL
1	G	56	LEU
1	G	70	MET
1	G	90	THR
1	G	100	ASN
1	G	108	LEU
1	G	109	LEU
1	G	111	ARG
1	G	117	LYS
1	G	127	SER
1	G	133	SER
1	G	137	SER
1	G	144	SER
1	G	146	SER
1	G	149	ARG
1	G	152	VAL
1	G	163	THR
1	G	194	LEU
1	G	197	ASN
1	G	207	SER
1	G	213	LEU
1	G	214	VAL
1	G	221	SER
1	G	235	THR
1	G	261	VAL
1	G	263	LYS
1	G	265	ASP
1	G	277	ASN

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Mol	Chain	Res	Type
1	G	284	THR
1	G	292	SER
1	G	293	MET
1	G	302	THR
1	G	310	VAL
1	G	312	SER
1	G	319	THR
2	H	336	LEU
2	H	356	TYR
2	H	362	ASN
2	H	383	THR
2	H	392	LYS
2	H	398	GLU
2	H	400	VAL
2	H	412	GLU
2	H	418	MET
2	H	423	LEU
2	H	425	VAL
2	H	427	THR
2	H	432	LEU
2	H	437	GLU
2	H	458	LEU
2	H	463	ASN
2	H	467	LEU
2	H	477	LYS
2	H	479	ASP
2	H	487	ARG
2	H	490	THR
2	H	494	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	88	ASN
1	A	100	ASN
1	A	196	GLN
2	B	362	ASN
2	B	476	HIS
1	C	12	HIS
1	C	91	ASN
1	C	186	ASN

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Mol	Chain	Res	Type
1	C	196	GLN
2	D	360	HIS
2	D	413	ASN
2	D	476	HIS
2	D	480	ASN
2	D	488	ASN
1	E	12	HIS
1	E	88	ASN
1	E	100	ASN
1	E	119	GLN
1	E	196	GLN
2	F	413	ASN
2	F	476	HIS
2	F	488	ASN
1	G	12	HIS
1	G	100	ASN
1	G	119	GLN
1	G	196	GLN
2	H	413	ASN
2	H	476	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	GAL	I	1	3	12,12,12	1.04	0	17,17,17	2.35	7 (41%)
3	SIA	I	2	3	20,20,21	0.56	0	21,28,31	0.82	1 (4%)
3	GAL	J	1	3	12,12,12	1.02	0	17,17,17	1.85	5 (29%)
3	SIA	J	2	3	20,20,21	0.56	0	21,28,31	0.82	2 (9%)

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	GAL	O2-C2-C3	-5.71	96.92	110.38
3	J	1	GAL	O3-C3-C4	3.47	118.54	110.38
3	I	1	GAL	O5-C5-C6	3.25	114.49	106.44
3	I	1	GAL	C4-C3-C2	3.20	116.44	110.83
3	J	1	GAL	O1-C1-C2	3.10	117.99	108.98
3	I	1	GAL	C1-C2-C3	3.07	116.62	110.36
3	I	1	GAL	O3-C3-C4	2.75	116.85	110.38
3	J	1	GAL	O5-C5-C4	-2.70	104.83	109.70
3	J	1	GAL	O1-C1-O5	-2.68	102.44	110.41
3	I	1	GAL	O2-C2-C1	2.47	114.94	109.25
3	J	1	GAL	O2-C2-C1	2.44	114.88	109.25
3	I	1	GAL	C1-O5-C5	2.44	118.36	113.65
3	I	2	SIA	O1B-C1-C2	2.22	118.49	112.71
3	J	2	SIA	O1B-C1-C2	2.22	118.48	112.71
3	J	2	SIA	O1A-C1-C2	-2.01	118.52	122.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

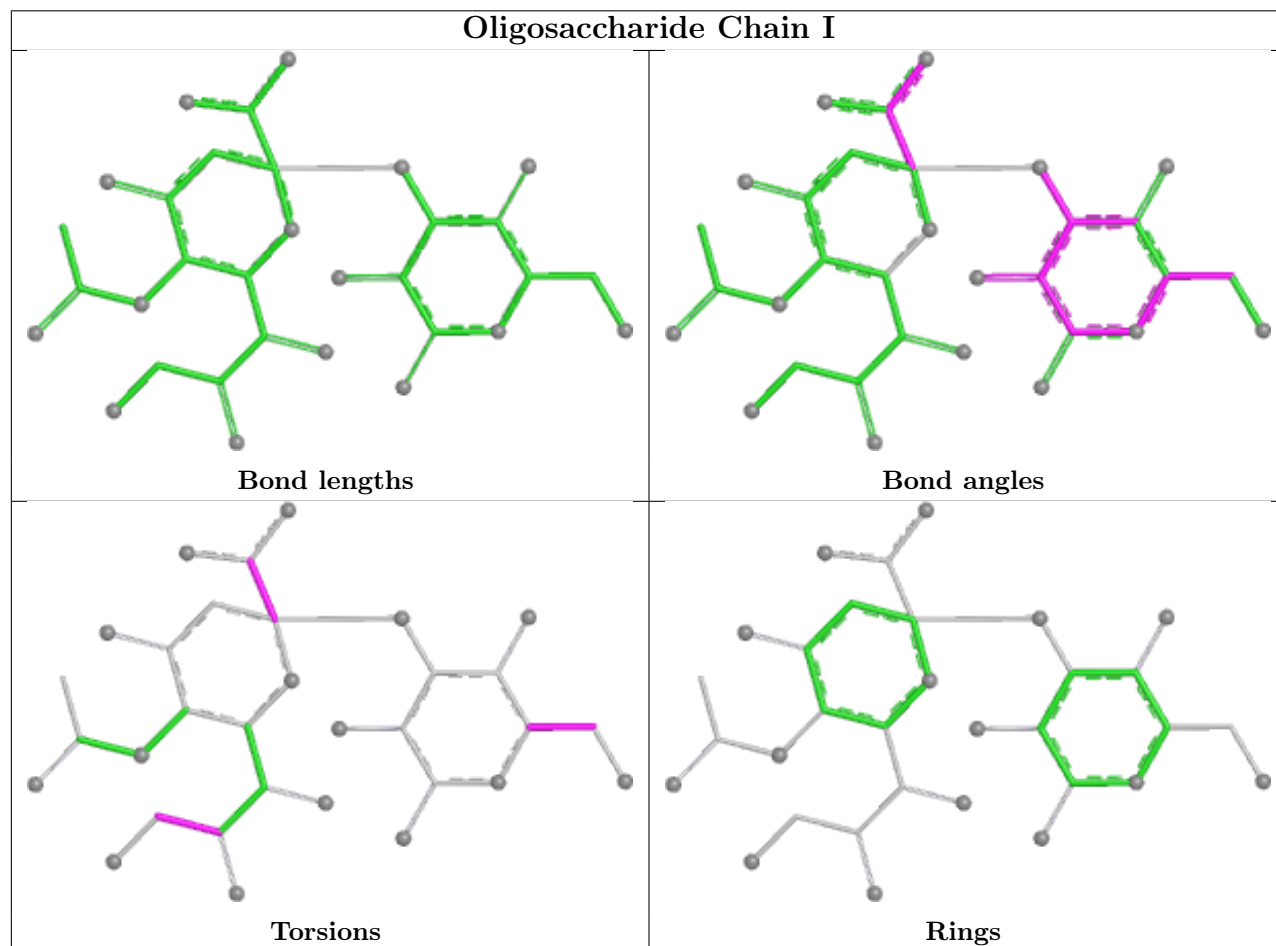
Mol	Chain	Res	Type	Atoms
3	J	1	GAL	O5-C5-C6-O6
3	J	2	SIA	O8-C8-C9-O9
3	I	1	GAL	C4-C5-C6-O6
3	J	1	GAL	C4-C5-C6-O6
3	I	1	GAL	O5-C5-C6-O6
3	J	2	SIA	C7-C8-C9-O9
3	I	2	SIA	O1A-C1-C2-O6
3	I	2	SIA	O8-C8-C9-O9
3	I	2	SIA	C7-C8-C9-O9

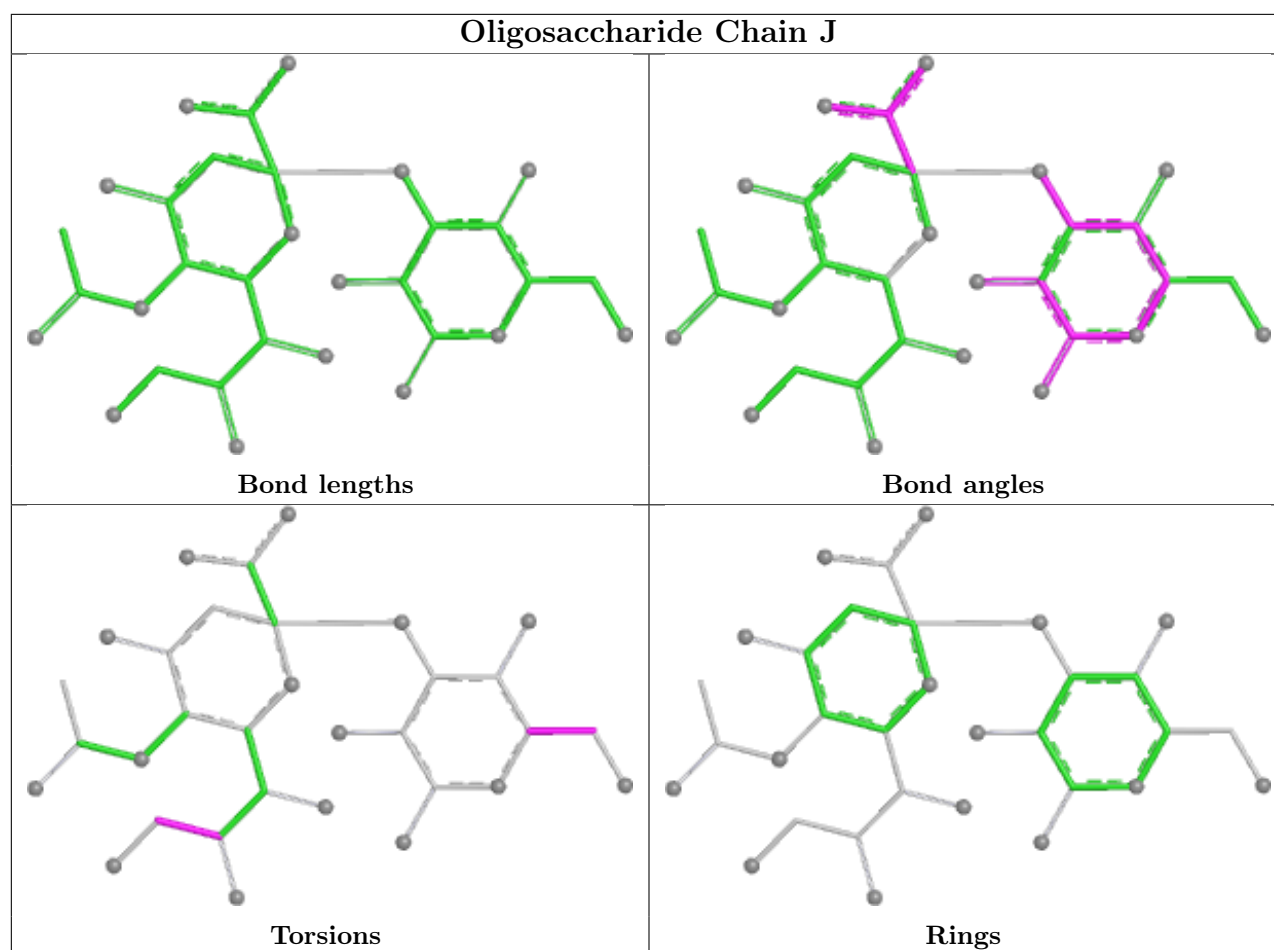
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	SIA	3	0
3	I	2	SIA	2	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	A	601	1	14,14,15	0.71	0	17,19,21	1.69	5 (29%)
4	NAG	C	601	1	14,14,15	1.18	2 (14%)	17,19,21	2.29	8 (47%)

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	A	601	1	-	3/6/23/26	0/1/1/1
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	NAG	O5-C1	-2.57	1.39	1.43
4	C	601	NAG	O5-C5	-2.00	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C2-N2-C7	-5.23	115.89	122.90
4	C	601	NAG	C1-O5-C5	3.66	117.09	112.19
4	C	601	NAG	O5-C1-C2	3.47	116.67	111.29
4	A	601	NAG	O4-C4-C5	3.13	117.03	109.32
4	A	601	NAG	C3-C4-C5	-2.81	105.14	110.23
4	C	601	NAG	C4-C3-C2	-2.75	106.99	111.02
4	C	601	NAG	C3-C4-C5	-2.72	105.30	110.23
4	A	601	NAG	C1-C2-N2	-2.71	106.16	110.43
4	C	601	NAG	C1-C2-N2	-2.65	106.25	110.43
4	C	601	NAG	O3-C3-C4	2.62	116.55	110.38
4	A	601	NAG	C2-N2-C7	-2.26	119.87	122.90
4	A	601	NAG	C1-O5-C5	2.14	115.05	112.19
4	C	601	NAG	O3-C3-C2	2.13	113.83	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	NAG	O5-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	2	0

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	321/321 (100%)	-1.25	0 100 100	17, 41, 84, 122	0
1	C	321/321 (100%)	-1.26	0 100 100	16, 41, 87, 131	0
1	E	321/321 (100%)	-0.40	0 100 100	65, 120, 189, 261	0
1	G	321/321 (100%)	-0.45	1 (0%) 90 79	58, 117, 187, 236	0
2	B	164/164 (100%)	-0.96	0 100 100	22, 85, 126, 140	0
2	D	164/164 (100%)	-0.92	0 100 100	23, 84, 127, 150	0
2	F	164/164 (100%)	0.07	2 (1%) 76 55	85, 165, 241, 300	0
2	H	164/164 (100%)	0.09	3 (1%) 67 44	82, 161, 228, 304	0
All	All	1940/1940 (100%)	-0.70	6 (0%) 90 79	16, 94, 193, 304	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	ILE	2.8
2	F	454	ASP	2.6
2	F	443	ASP	2.4
2	H	486	ILE	2.2
2	H	452	LEU	2.2
2	H	475	TYR	2.2

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

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

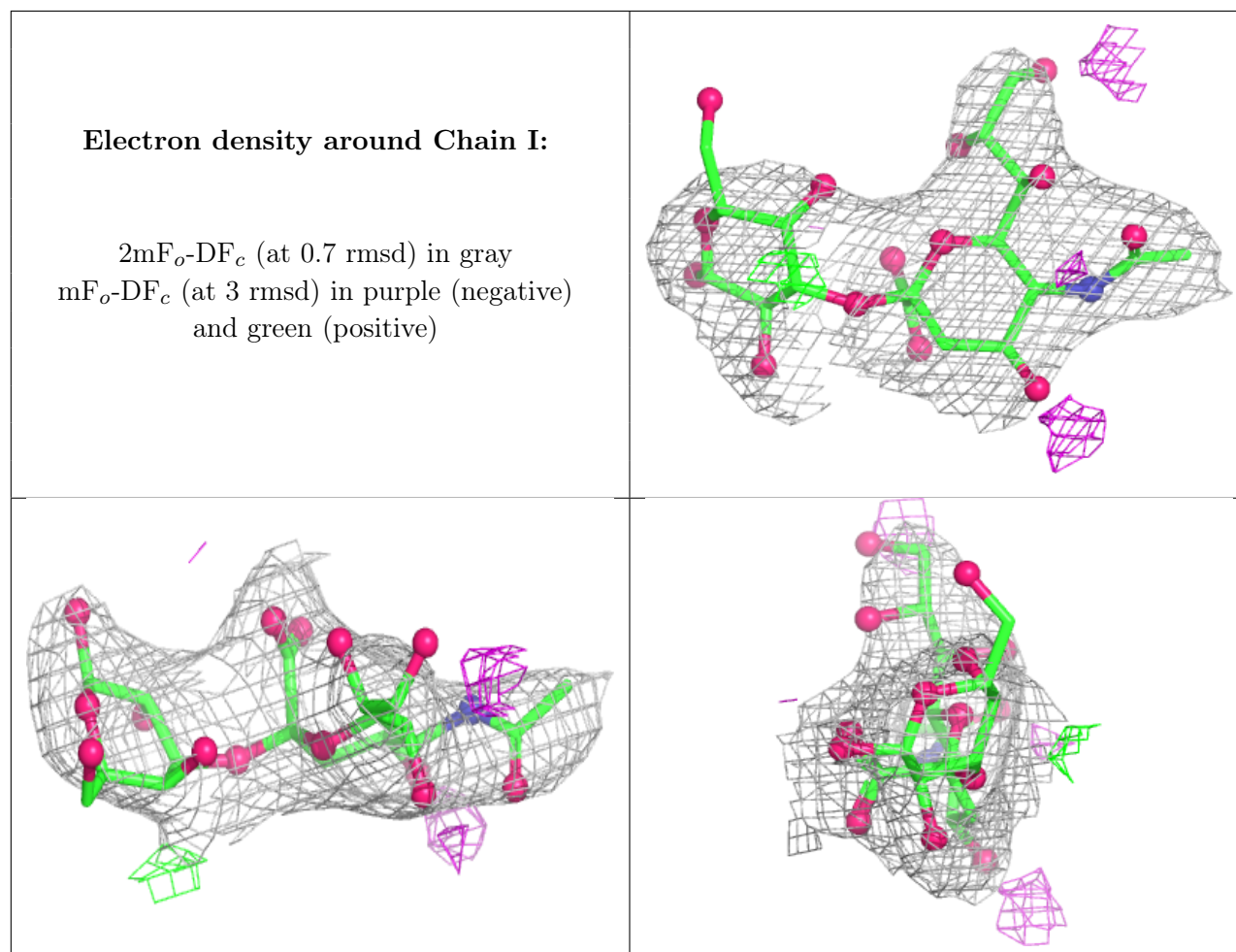
6.3 Carbohydrates [i](#)

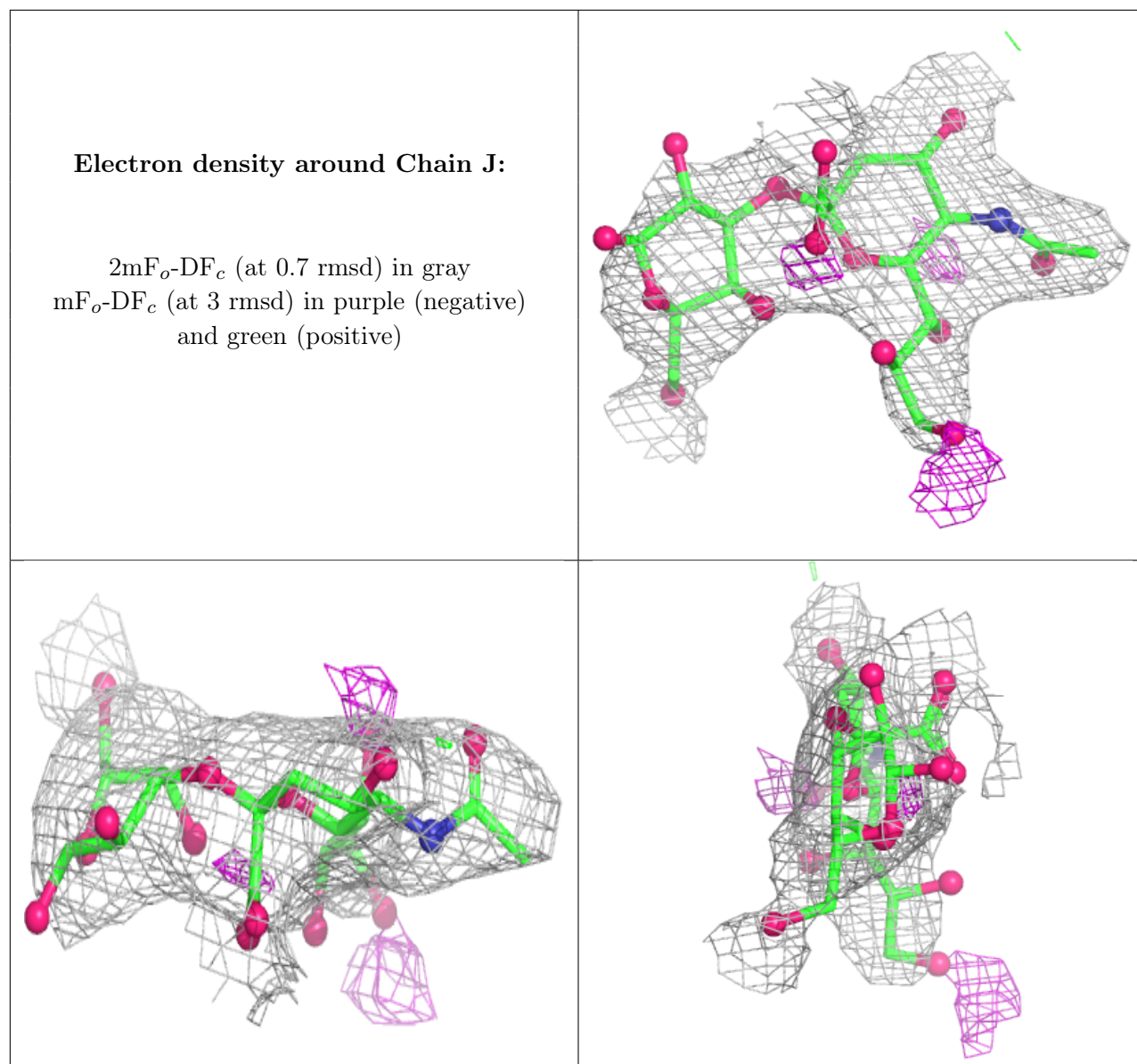
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	GAL	J	1	12/12	0.94	0.09	62,69,85,92	0
3	GAL	I	1	12/12	0.97	0.07	60,64,85,87	0
3	SIA	I	2	20/21	0.99	0.05	31,45,55,55	0
3	SIA	J	2	20/21	0.99	0.05	32,45,56,58	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 ⓘ

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
4	NAG	C	601	14/15	0.97	0.05	37,51,67,71	0
4	NAG	A	601	14/15	0.98	0.04	39,55,63,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.