



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:32 am GMT

PDB ID : 4K67  
Title : Structure of an airborne transmissible avian influenza H5 hemagglutinin mutant from the influenza virus A/Indonesia/5/2005 complexed with human receptor analog LSTc  
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Gao, G.F.  
Deposited on : 2013-04-15  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

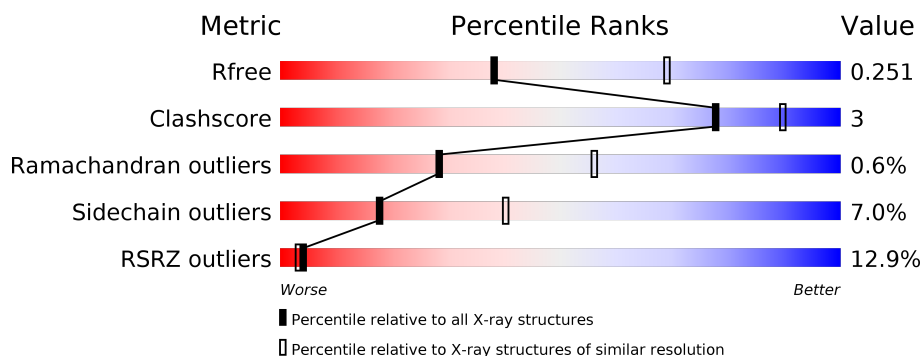
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	321	<div> <div>%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	E	321	<div> <div>6%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	G	321	<div> <div>6%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	164	<div> <div>18%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	D	164	<div> <div>18%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	164	<div><div>44%</div><div><div></div><div></div><div></div></div><div>84%</div><div>14%</div><div></div></div>
2	H	164	<div><div>44%</div><div><div></div><div></div><div></div></div><div>85%</div><div>13%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15692 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			

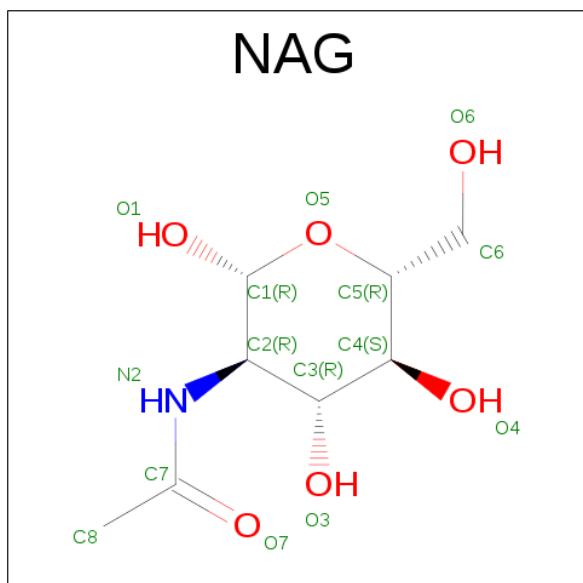
There are 20 discrepancies between the modelled and reference sequences:

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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			32	17	1	14		
4	C	2	Total	C	N	O	0	0
			32	17	1	14		

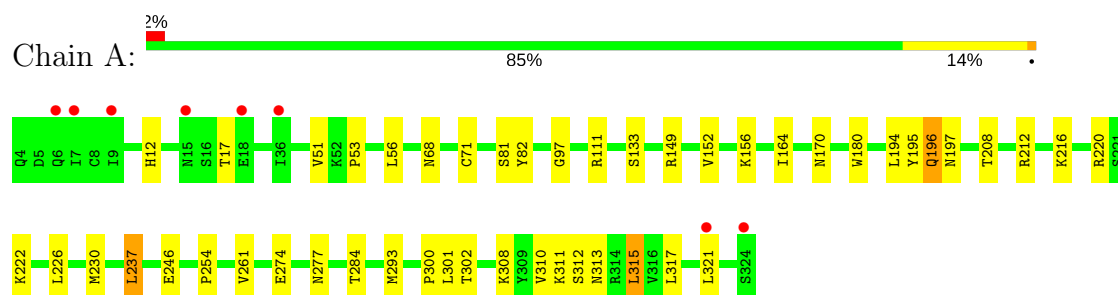
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	3	Total	C	N	O	0	0
			46	25	2	19		
5	G	3	Total	C	N	O	0	0
			46	25	2	19		

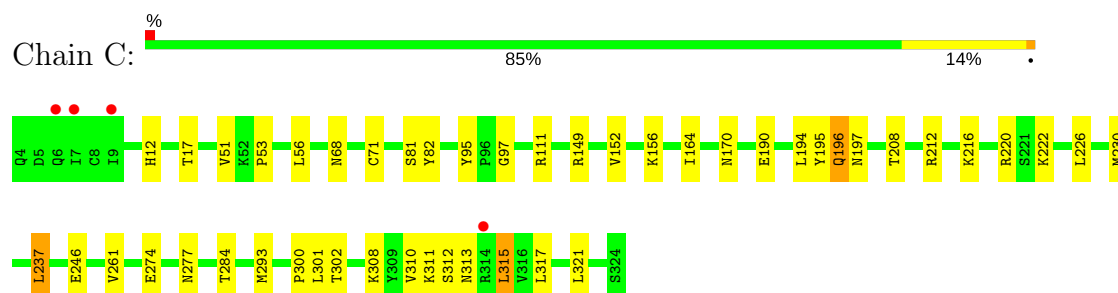
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

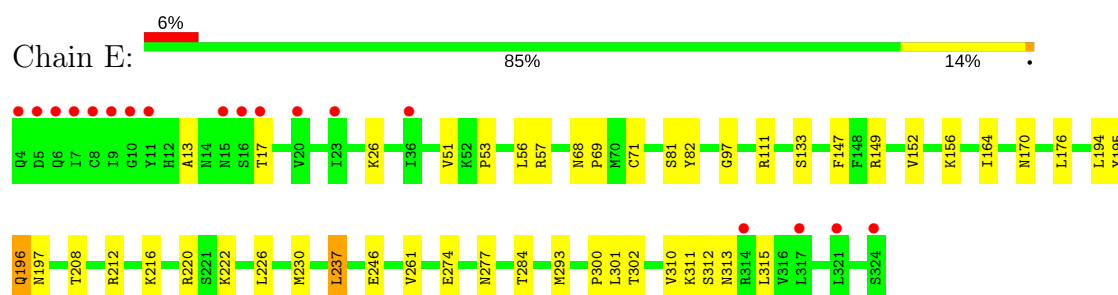
#### • Molecule 1: Hemagglutinin



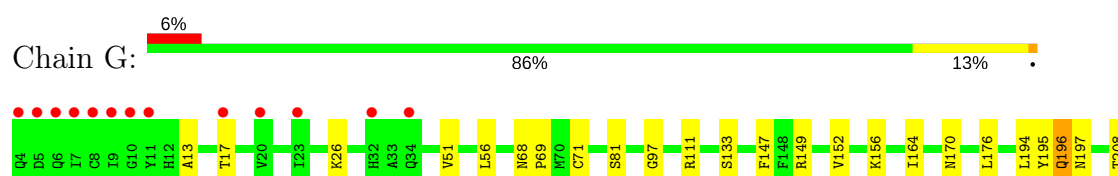
#### • Molecule 1: Hemagglutinin



#### • Molecule 1: Hemagglutinin

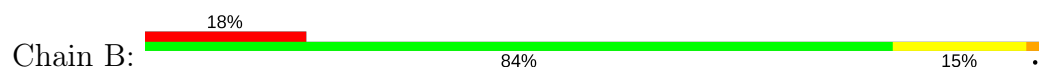


#### • Molecule 1: Hemagglutinin

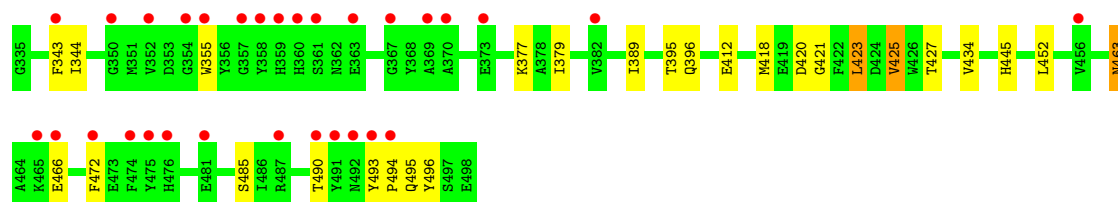
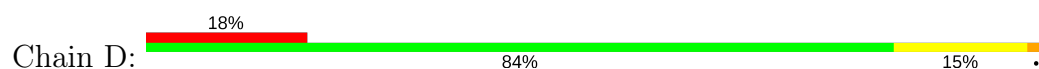




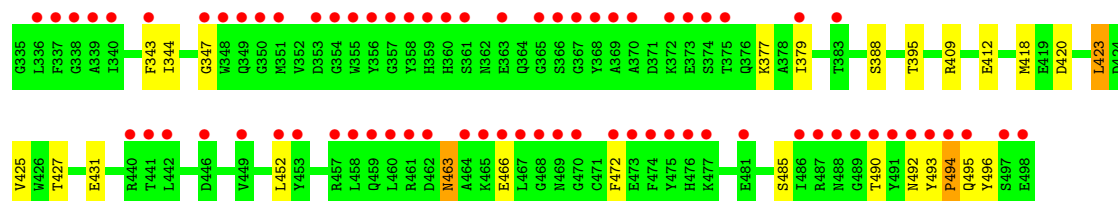
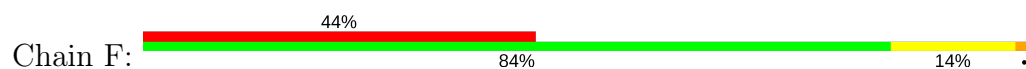
• Molecule 2: Hemagglutinin



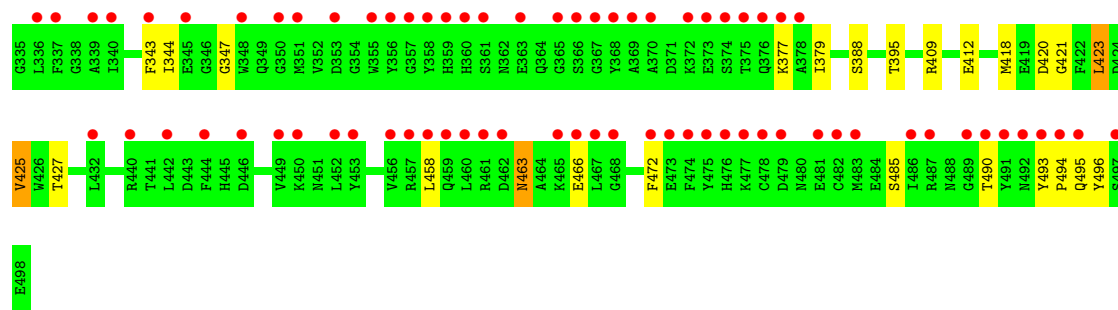
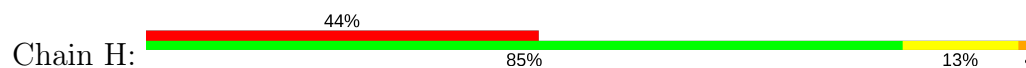
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.63Å 70.63Å 494.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 2.70 49.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.12-2.70) 95.3 (49.12-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.227 , 0.255 0.218 , 0.251	Depositor DCC
$R_{free}$ test set	3626 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.437 for -h,-k,l 0.069 for h,-h-k,-l 0.062 for -k,-h,-l	Xtriage
Reported twinning fraction	0.221 for -h,-k,l	Depositor
Outliers	0 of 72276 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.5285e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: SIA, GAL, 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	0.32	0/2604	0.51	0/3539
1	C	0.32	0/2604	0.51	0/3539
1	E	0.33	0/2604	0.68	3/3539 (0.1%)
1	G	0.32	0/2604	0.51	0/3539
2	B	0.27	0/1355	0.43	0/1823
2	D	0.27	0/1355	0.43	0/1823
2	F	0.27	0/1355	0.43	0/1823
2	H	0.27	0/1355	0.44	0/1823
All	All	0.31	0/15836	0.52	3/21448 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	ARG	NE-CZ-NH1	-19.37	110.61	120.30
1	E	57	ARG	NE-CZ-NH2	15.61	128.10	120.30
1	E	57	ARG	CD-NE-CZ	10.20	137.88	123.60

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	22	0
1	C	2542	0	2483	23	0
1	E	2542	0	2483	18	1
1	G	2542	0	2483	18	1
2	B	1328	0	1231	12	0
2	D	1328	0	1231	13	0
2	F	1328	0	1231	9	1
2	H	1328	0	1231	8	1
3	A	14	0	13	0	0
3	C	14	0	13	0	0
3	E	14	0	13	0	0
3	G	14	0	13	0	0
4	A	32	0	27	1	0
4	C	32	0	27	2	0
5	E	46	0	39	1	0
5	G	46	0	39	1	0
All	All	15692	0	15040	104	2

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 3.

All (104) 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:216:LYS:O	1:E:220:ARG:NH2	2.22	0.73
1:A:216:LYS:O	1:A:220:ARG:NH2	2.23	0.72
1:C:216:LYS:O	1:C:220:ARG:NH2	2.24	0.71
1:G:216:LYS:O	1:G:220:ARG:NH2	2.25	0.70
1:C:95:TYR:OH	4:C:602:SIA:H91	2.00	0.62
1:G:51:VAL:HG13	1:G:81:SER:HB3	1.83	0.61
1:A:51:VAL:HG13	1:A:81:SER:HB3	1.83	0.60
1:E:51:VAL:HG13	1:E:81:SER:HB3	1.84	0.59
1:C:51:VAL:HG13	1:C:81:SER:HB3	1.84	0.58
1:C:12:HIS:HB2	2:D:355:TRP:HA	1.86	0.57
1:C:317:LEU:HD21	2:D:389:ILE:HD12	1.86	0.56
1:A:317:LEU:HD21	2:B:389:ILE:HD12	1.88	0.55
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.43	0.54
1:G:310:VAL:HG12	1:G:312:SER:H	1.75	0.52
1:A:12:HIS:HB2	2:B:355:TRP:HA	1.91	0.52
1:G:195:TYR:O	1:G:197:ASN:N	2.41	0.52
1:G:170:ASN:HB2	1:G:237:LEU:HD13	1.92	0.52
1:C:170:ASN:HB2	1:C:237:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLY:HA3	1:A:230:MET:O	2.11	0.51
1:E:170:ASN:HB2	1:E:237:LEU:HD13	1.93	0.51
1:A:321:LEU:HB3	2:B:445:HIS:CD2	2.46	0.51
1:E:310:VAL:HG12	1:E:312:SER:H	1.75	0.50
1:E:312:SER:OG	2:F:431:GLU:OE2	2.19	0.50
1:A:310:VAL:HG12	1:A:312:SER:H	1.75	0.50
1:G:97:GLY:HA3	1:G:230:MET:O	2.12	0.50
1:C:195:TYR:O	1:C:197:ASN:N	2.43	0.49
1:E:133:SER:O	5:E:602:SIA:H113	2.13	0.49
1:C:310:VAL:HG12	1:C:312:SER:H	1.75	0.49
1:E:164:ILE:O	1:E:246:GLU:HA	2.12	0.49
2:B:343:PHE:CD1	2:B:344:ILE:HG13	2.48	0.49
1:C:311:LYS:HE3	2:D:423:LEU:HD11	1.92	0.49
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.94	0.49
1:A:311:LYS:HE3	2:B:423:LEU:HD11	1.93	0.48
1:C:97:GLY:HA3	1:C:230:MET:O	2.13	0.48
1:A:222:LYS:HA	1:A:226:LEU:O	2.14	0.48
2:F:343:PHE:CD1	2:F:344:ILE:HG13	2.49	0.48
1:E:97:GLY:HA3	1:E:230:MET:O	2.14	0.48
2:B:463:ASN:OD1	2:B:463:ASN:N	2.47	0.48
1:C:164:ILE:O	1:C:246:GLU:HA	2.13	0.48
2:D:343:PHE:CD1	2:D:344:ILE:HG13	2.48	0.48
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.48
1:A:170:ASN:HB2	1:A:237:LEU:HD13	1.96	0.48
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.53	0.47
1:A:300:PRO:HG2	1:A:301:LEU:HD12	1.96	0.47
2:F:463:ASN:OD1	2:F:463:ASN:N	2.47	0.47
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.96	0.47
1:G:68:ASN:HB3	1:G:71:CYS:SG	2.54	0.47
1:A:164:ILE:O	1:A:246:GLU:HA	2.13	0.47
1:G:311:LYS:HE3	2:H:423:LEU:HD11	1.97	0.47
1:C:300:PRO:HG2	1:C:301:LEU:HD12	1.97	0.47
2:H:343:PHE:CD1	2:H:344:ILE:HG13	2.49	0.47
1:C:317:LEU:HD13	2:D:434:VAL:HG22	1.97	0.47
1:E:311:LYS:HE3	2:F:423:LEU:HD11	1.97	0.47
2:D:463:ASN:OD1	2:D:463:ASN:N	2.47	0.47
1:G:133:SER:O	5:G:602:SIA:H113	2.14	0.47
1:C:315:LEU:HD22	2:D:434:VAL:HG21	1.98	0.46
1:E:68:ASN:HB3	1:E:71:CYS:SG	2.56	0.46
1:G:300:PRO:HG2	1:G:301:LEU:HD12	1.97	0.46
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:PRO:HG2	1:E:301:LEU:HD12	1.97	0.46
2:H:463:ASN:N	2:H:463:ASN:OD1	2.47	0.46
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.97	0.46
1:E:195:TYR:O	1:E:197:ASN:N	2.44	0.45
1:E:13:ALA:HB2	2:F:347:GLY:HA3	1.99	0.45
1:C:222:LYS:HA	1:C:226:LEU:O	2.16	0.45
1:C:315:LEU:HA	1:C:315:LEU:HD23	1.82	0.45
1:A:315:LEU:HD22	2:B:434:VAL:HG21	1.99	0.45
1:A:308:LYS:HB3	2:B:396:GLN:NE2	2.31	0.45
1:C:190:GLU:OE2	4:C:602:SIA:O9	2.35	0.45
1:G:222:LYS:HA	1:G:226:LEU:O	2.16	0.45
1:A:317:LEU:HD13	2:B:434:VAL:HG22	1.98	0.44
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.56	0.44
1:E:222:LYS:HA	1:E:226:LEU:O	2.18	0.44
2:B:493:TYR:O	2:B:495:GLN:N	2.51	0.43
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.89	0.43
1:G:317:LEU:HA	1:G:317:LEU:HD12	1.87	0.43
1:E:176:LEU:HD23	1:E:176:LEU:HA	1.86	0.43
1:C:308:LYS:HB3	2:D:396:GLN:NE2	2.32	0.43
1:A:195:TYR:O	1:A:197:ASN:N	2.44	0.43
2:D:493:TYR:O	2:D:495:GLN:N	2.51	0.42
2:D:466:GLU:HA	2:D:472:PHE:HD2	1.84	0.42
2:F:452:LEU:HD12	2:F:452:LEU:HA	1.90	0.42
1:G:176:LEU:HA	1:G:176:LEU:HD23	1.86	0.42
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.85	0.42
2:B:466:GLU:HA	2:B:472:PHE:HD2	1.84	0.42
2:H:493:TYR:O	2:H:495:GLN:N	2.53	0.42
2:F:493:TYR:O	2:F:495:GLN:N	2.53	0.42
1:A:133:SER:O	4:A:602:SIA:H113	2.19	0.42
2:F:466:GLU:HA	2:F:472:PHE:HD2	1.85	0.42
2:D:421:GLY:O	2:D:425:VAL:HG13	2.20	0.41
2:B:421:GLY:O	2:B:425:VAL:HG13	2.20	0.41
1:G:69:PRO:HG3	1:G:147:PHE:O	2.20	0.41
1:C:53:PRO:HB3	1:C:82:TYR:CZ	2.55	0.41
1:G:315:LEU:HA	1:G:315:LEU:HD23	1.82	0.41
1:G:13:ALA:HB2	2:H:347:GLY:HA3	2.02	0.41
2:H:421:GLY:O	2:H:425:VAL:HG13	2.21	0.41
2:H:466:GLU:HA	2:H:472:PHE:HD2	1.85	0.41
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.93	0.41
1:A:180:TRP:HB3	1:A:254:PRO:HG3	2.03	0.40
1:A:53:PRO:HB3	1:A:82:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PRO:HB3	1:E:82:TYR:CZ	2.57	0.40
1:E:69:PRO:HG3	1:E:147:PHE:O	2.21	0.40
2:H:458:LEU:HA	2:H:458:LEU:HD13	1.94	0.40
2:F:492:ASN:OD1	2:F:494:PRO:HD2	2.22	0.40

All (2) 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:G:26:LYS:NZ	2:H:388:SER:OG[3_665]	2.06	0.14
1:E:26:LYS:NZ	2:F:388:SER:OG[3_655]	2.06	0.14

## 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%)	305 (96%)	13 (4%)	1 (0%)	44	73
1	C	319/321 (99%)	306 (96%)	12 (4%)	1 (0%)	44	73
1	E	319/321 (99%)	307 (96%)	11 (3%)	1 (0%)	44	73
1	G	319/321 (99%)	306 (96%)	12 (4%)	1 (0%)	44	73
2	B	162/164 (99%)	150 (93%)	10 (6%)	2 (1%)	15	37
2	D	162/164 (99%)	149 (92%)	11 (7%)	2 (1%)	15	37
2	F	162/164 (99%)	149 (92%)	11 (7%)	2 (1%)	15	37
2	H	162/164 (99%)	150 (93%)	10 (6%)	2 (1%)	15	37
All	All	1924/1940 (99%)	1822 (95%)	90 (5%)	12 (1%)	28	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	496	TYR
2	D	496	TYR
2	F	496	TYR
2	H	496	TYR
2	B	494	PRO
2	D	494	PRO
2	F	494	PRO
2	H	494	PRO
1	A	196	GLN
1	C	196	GLN
1	G	196	GLN
1	E	196	GLN

### 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%)	271 (94%)	17 (6%)	23	49
1	C	288/288 (100%)	271 (94%)	17 (6%)	23	49
1	E	288/288 (100%)	271 (94%)	17 (6%)	23	49
1	G	288/288 (100%)	271 (94%)	17 (6%)	23	49
2	B	140/140 (100%)	127 (91%)	13 (9%)	10	24
2	D	140/140 (100%)	128 (91%)	12 (9%)	12	28
2	F	140/140 (100%)	127 (91%)	13 (9%)	10	24
2	H	140/140 (100%)	127 (91%)	13 (9%)	10	24
All	All	1712/1712 (100%)	1593 (93%)	119 (7%)	18	40

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	56	LEU
1	A	111	ARG
1	A	149	ARG

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Mol	Chain	Res	Type
1	A	152	VAL
1	A	194	LEU
1	A	208	THR
1	A	212	ARG
1	A	237	LEU
1	A	261	VAL
1	A	274	GLU
1	A	277	ASN
1	A	284	THR
1	A	293	MET
1	A	302	THR
1	A	313	ASN
1	A	315	LEU
2	B	377	LYS
2	B	379	ILE
2	B	395	THR
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	463	ASN
2	B	485	SER
2	B	490	THR
2	B	498	GLU
1	C	17	THR
1	C	56	LEU
1	C	111	ARG
1	C	149	ARG
1	C	152	VAL
1	C	194	LEU
1	C	208	THR
1	C	212	ARG
1	C	237	LEU
1	C	261	VAL
1	C	274	GLU
1	C	277	ASN
1	C	284	THR
1	C	293	MET
1	C	302	THR
1	C	313	ASN

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Mol	Chain	Res	Type
1	C	315	LEU
2	D	377	LYS
2	D	379	ILE
2	D	395	THR
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	463	ASN
2	D	485	SER
2	D	490	THR
1	E	17	THR
1	E	56	LEU
1	E	111	ARG
1	E	149	ARG
1	E	152	VAL
1	E	194	LEU
1	E	208	THR
1	E	212	ARG
1	E	237	LEU
1	E	261	VAL
1	E	274	GLU
1	E	277	ASN
1	E	284	THR
1	E	293	MET
1	E	302	THR
1	E	313	ASN
1	E	315	LEU
2	F	377	LYS
2	F	379	ILE
2	F	395	THR
2	F	409	ARG
2	F	412	GLU
2	F	418	MET
2	F	420	ASP
2	F	423	LEU
2	F	425	VAL
2	F	427	THR
2	F	463	ASN
2	F	485	SER

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Mol	Chain	Res	Type
2	F	490	THR
1	G	17	THR
1	G	56	LEU
1	G	111	ARG
1	G	149	ARG
1	G	152	VAL
1	G	194	LEU
1	G	208	THR
1	G	212	ARG
1	G	237	LEU
1	G	261	VAL
1	G	274	GLU
1	G	277	ASN
1	G	284	THR
1	G	293	MET
1	G	302	THR
1	G	313	ASN
1	G	315	LEU
2	H	377	LYS
2	H	379	ILE
2	H	395	THR
2	H	409	ARG
2	H	412	GLU
2	H	418	MET
2	H	420	ASP
2	H	423	LEU
2	H	425	VAL
2	H	427	THR
2	H	463	ASN
2	H	485	SER
2	H	490	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	396	GLN
2	D	396	GLN
1	E	12	HIS
2	F	396	GLN
1	G	12	HIS
2	H	396	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 ⓘ

10 carbohydrates 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	SIA	A	602	4	17,20,21	3.71	6 (35%)	19,28,31	2.52	4 (21%)
4	GAL	A	603	4	12,12,12	0.50	0	17,17,17	1.27	1 (5%)
4	SIA	C	602	4	17,20,21	3.65	8 (47%)	19,28,31	2.34	4 (21%)
4	GAL	C	603	4	12,12,12	0.46	0	17,17,17	0.93	1 (5%)
5	SIA	E	602	5	17,20,21	3.62	7 (41%)	19,28,31	2.55	4 (21%)
5	GAL	E	603	5	11,11,12	0.64	0	13,15,17	1.65	1 (7%)
5	NAG	E	604	5	15,15,15	0.41	0	21,21,21	1.22	2 (9%)
5	SIA	G	602	5	17,20,21	3.62	7 (41%)	19,28,31	2.55	5 (26%)
5	GAL	G	603	5	11,11,12	0.68	0	13,15,17	1.49	1 (7%)
5	NAG	G	604	5	15,15,15	0.41	0	21,21,21	0.79	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
4	SIA	A	602	4	-	0/14/34/38	0/1/1/1
4	GAL	A	603	4	-	0/2/22/22	0/1/1/1
4	SIA	C	602	4	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	C	603	4	-	0/2/22/22	0/1/1/1
5	SIA	E	602	5	-	0/14/34/38	0/1/1/1
5	GAL	E	603	5	-	0/2/19/22	0/1/1/1
5	NAG	E	604	5	-	0/6/26/26	0/1/1/1
5	SIA	G	602	5	-	0/14/34/38	0/1/1/1
5	GAL	G	603	5	-	0/2/19/22	0/1/1/1
5	NAG	G	604	5	-	0/6/26/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	SIA	C4-C5	-10.70	1.42	1.53
4	C	602	SIA	C4-C5	-10.18	1.43	1.53
5	E	602	SIA	C4-C5	-9.78	1.43	1.53
5	G	602	SIA	C4-C5	-9.54	1.44	1.53
5	G	602	SIA	C7-C6	-8.37	1.42	1.52
5	E	602	SIA	C7-C6	-8.30	1.42	1.52
4	C	602	SIA	C7-C6	-7.98	1.42	1.52
4	A	602	SIA	C7-C6	-7.89	1.43	1.52
5	G	602	SIA	O7-C7	-2.36	1.37	1.43
4	A	602	SIA	O8-C8	-2.31	1.38	1.43
4	C	602	SIA	O8-C8	-2.18	1.38	1.43
4	C	602	SIA	O7-C7	-2.15	1.38	1.43
4	A	602	SIA	O7-C7	-2.13	1.38	1.43
5	E	602	SIA	O7-C7	-2.12	1.38	1.43
4	C	602	SIA	O6-C2	-2.08	1.38	1.43
5	E	602	SIA	C5-N5	2.05	1.49	1.45
4	C	602	SIA	C5-N5	2.18	1.49	1.45
5	E	602	SIA	C3-C2	2.18	1.56	1.52
5	G	602	SIA	C5-N5	2.30	1.49	1.45
5	G	602	SIA	C3-C2	2.49	1.56	1.52
4	C	602	SIA	O6-C6	3.56	1.49	1.43
4	A	602	SIA	O6-C6	3.61	1.49	1.43
5	E	602	SIA	O6-C6	3.69	1.49	1.43
5	G	602	SIA	O6-C6	3.77	1.49	1.43
4	C	602	SIA	C10-N5	4.02	1.49	1.34
4	A	602	SIA	C10-N5	4.17	1.49	1.34
5	E	602	SIA	C10-N5	4.18	1.49	1.34
5	G	602	SIA	C10-N5	4.27	1.50	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	602	SIA	O6-C2-C3	-7.69	95.97	109.82
4	A	602	SIA	O6-C2-C3	-7.52	96.27	109.82
5	E	602	SIA	O6-C2-C3	-7.33	96.63	109.82
4	C	602	SIA	O6-C2-C3	-6.84	97.51	109.82
5	E	603	GAL	C1-O5-C5	-5.21	104.98	112.17
5	G	603	GAL	C1-O5-C5	-5.09	105.16	112.17
5	E	602	SIA	C8-C7-C6	-4.11	105.05	113.04
4	A	602	SIA	C8-C7-C6	-3.33	106.58	113.04
5	G	602	SIA	C8-C7-C6	-2.80	107.59	113.04
4	C	602	SIA	C8-C7-C6	-2.67	107.84	113.04
4	A	603	GAL	C6-C5-C4	-2.59	106.93	113.00
4	C	603	GAL	C6-C5-C4	-2.47	107.22	113.00
5	E	604	NAG	O5-C1-C2	2.03	111.56	109.52
5	G	602	SIA	C3-C4-C5	2.31	114.25	111.46
4	C	602	SIA	C3-C4-C5	2.56	114.56	111.46
5	E	602	SIA	C3-C4-C5	2.93	115.01	111.46
5	G	602	SIA	O9-C9-C8	3.05	117.83	111.11
5	E	604	NAG	C1-C2-C3	3.10	114.78	110.54
4	A	602	SIA	C3-C4-C5	3.46	115.64	111.46
5	G	602	SIA	C4-C3-C2	4.63	118.44	109.75
4	A	602	SIA	C4-C3-C2	5.05	119.23	109.75
4	C	602	SIA	C4-C3-C2	5.07	119.26	109.75
5	E	602	SIA	C4-C3-C2	5.26	119.62	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	SIA	1	0
4	C	602	SIA	2	0
5	E	602	SIA	1	0
5	G	602	SIA	1	0

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	NAG	A	601	1	14,14,15	0.48	0	15,19,21	1.34	2 (13%)
3	NAG	C	601	1	14,14,15	0.46	0	15,19,21	1.35	2 (13%)
3	NAG	E	601	1	14,14,15	0.54	0	15,19,21	1.08	1 (6%)
3	NAG	G	601	1	14,14,15	0.56	0	15,19,21	0.78	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	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	C2-N2-C7	-2.44	119.38	122.94
3	C	601	NAG	C2-N2-C7	-2.44	119.39	122.94
3	E	601	NAG	C1-C2-N2	-2.12	106.87	110.49
3	C	601	NAG	C1-O5-C5	3.20	116.58	112.17
3	A	601	NAG	C1-O5-C5	3.39	116.84	112.17

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/321 (100%)	0.12	8 (2%) 58 58	19, 46, 102, 171	0
1	C	321/321 (100%)	0.08	4 (1%) 79 80	18, 46, 99, 165	0
1	E	321/321 (100%)	0.29	18 (5%) 25 23	18, 48, 130, 244	0
1	G	321/321 (100%)	0.26	18 (5%) 25 23	22, 46, 124, 234	0
2	B	164/164 (100%)	0.98	29 (17%) 2 1	27, 103, 164, 204	0
2	D	164/164 (100%)	1.04	30 (18%) 1 1	28, 103, 167, 189	0
2	F	164/164 (100%)	2.26	72 (43%) 0 0	26, 144, 214, 255	0
2	H	164/164 (100%)	2.40	72 (43%) 0 0	28, 147, 223, 253	0
All	All	1940/1940 (100%)	0.69	251 (12%) 4 3	18, 58, 177, 255	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	356	TYR	11.6
1	E	10	GLY	10.8
1	G	10	GLY	10.7
2	H	366	SER	9.4
2	F	491	TYR	9.4
2	F	465	LYS	9.0
2	H	493	TYR	8.8
2	H	494	PRO	8.5
2	F	475	TYR	8.1
2	H	465	LYS	8.1
2	H	472	PHE	7.8
2	F	493	TYR	7.8
2	H	491	TYR	7.7
2	H	355	TRP	7.7
2	F	357	GLY	7.6
1	E	6	GLN	7.5

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Mol	Chain	Res	Type	RSRZ
2	F	472	PHE	7.5
2	H	357	GLY	7.4
2	F	356	TYR	7.3
2	H	475	TYR	7.1
2	H	487	ARG	7.1
2	H	353	ASP	7.0
2	F	358	TYR	6.9
2	F	474	PHE	6.8
2	F	369	ALA	6.8
2	F	494	PRO	6.5
2	H	369	ALA	6.4
2	F	466	GLU	6.3
2	H	490	THR	6.3
2	H	468	GLY	6.2
2	F	492	ASN	6.2
2	F	366	SER	6.1
2	F	481	GLU	6.1
1	E	9	ILE	6.0
2	H	348	TRP	6.0
2	H	492	ASN	5.9
2	F	343	PHE	5.8
2	F	468	GLY	5.8
2	H	365	GLY	5.7
2	H	358	TYR	5.6
2	F	355	TRP	5.6
2	F	467	LEU	5.5
1	E	8	CYS	5.5
2	F	339	ALA	5.4
2	H	361	SER	5.4
2	H	466	GLU	5.4
2	H	467	LEU	5.3
2	H	363	GLU	5.3
2	F	462	ASP	5.3
2	H	473	GLU	5.2
2	F	360	HIS	5.2
2	D	361	SER	5.1
2	H	339	ALA	5.1
2	F	363	GLU	5.1
2	F	473	GLU	5.0
2	F	489	GLY	5.0
2	H	360	HIS	4.9
2	D	465	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
2	H	495	GLN	4.8
2	F	348	TRP	4.8
2	H	449	VAL	4.8
2	H	474	PHE	4.8
1	G	9	ILE	4.8
2	D	475	TYR	4.8
2	F	458	LEU	4.8
2	H	374	SER	4.7
2	H	481	GLU	4.6
2	D	481	GLU	4.6
2	F	446	ASP	4.5
2	F	460	LEU	4.5
2	F	490	THR	4.5
1	E	16	SER	4.4
2	D	492	ASN	4.3
2	F	372	LYS	4.3
2	H	489	GLY	4.3
2	H	359	HIS	4.2
2	H	367	GLY	4.2
1	G	4	GLN	4.2
2	H	372	LYS	4.2
2	D	487	ARG	4.1
2	F	476	HIS	4.1
2	F	487	ARG	4.1
2	H	370	ALA	4.1
1	E	17	THR	4.0
2	F	453	TYR	4.0
2	H	446	ASP	4.0
1	G	7	ILE	4.0
2	F	336	LEU	4.0
1	G	8	CYS	3.9
2	F	498	GLU	3.9
2	F	350	GLY	3.9
2	F	359	HIS	3.8
2	H	343	PHE	3.8
2	H	378	ALA	3.8
2	B	360	HIS	3.8
1	A	6	GLN	3.7
2	H	453	TYR	3.7
1	E	7	ILE	3.7
2	B	369	ALA	3.7
2	H	368	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	491	TYR	3.6
2	H	460	LEU	3.6
2	B	494	PRO	3.6
2	D	493	TYR	3.6
2	D	360	HIS	3.6
1	E	5	ASP	3.6
2	B	373	GLU	3.6
2	H	440	ARG	3.6
2	F	353	ASP	3.6
2	F	361	SER	3.6
2	H	373	GLU	3.6
2	H	337	PHE	3.6
2	B	487	ARG	3.5
2	H	482	CYS	3.5
1	G	320	GLY	3.5
2	B	363	GLU	3.5
2	D	367	GLY	3.5
2	F	338	GLY	3.5
1	G	17	THR	3.5
2	B	465	LYS	3.4
2	B	372	LYS	3.4
2	H	336	LEU	3.4
2	D	494	PRO	3.4
2	F	365	GLY	3.4
2	F	375	THR	3.4
2	B	481	GLU	3.4
2	F	374	SER	3.3
1	E	4	GLN	3.3
2	F	337	PHE	3.3
2	B	458	LEU	3.3
2	H	442	LEU	3.3
2	D	476	HIS	3.3
2	F	349	GLN	3.2
2	F	347	GLY	3.2
2	F	368	TYR	3.2
1	A	7	ILE	3.2
2	D	456	VAL	3.2
2	H	350	GLY	3.2
2	F	452	LEU	3.1
2	F	495	GLN	3.1
2	D	491	TYR	3.1
2	D	373	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	9	ILE	3.1
2	B	493	TYR	3.1
2	D	472	PHE	3.1
2	F	461	ARG	3.1
2	F	449	VAL	3.1
1	G	11	TYR	3.0
1	E	15	ASN	3.0
1	C	9	ILE	3.0
2	B	475	TYR	3.0
2	H	456	VAL	3.0
2	B	367	GLY	3.0
2	B	355	TRP	3.0
2	F	464	ALA	3.0
2	D	363	GLU	3.0
2	H	486	ILE	2.9
2	H	444	PHE	2.9
1	G	20	VAL	2.9
2	B	476	HIS	2.9
2	D	369	ALA	2.9
1	G	319	THR	2.9
2	H	497	SER	2.9
2	H	458	LEU	2.8
1	G	6	GLN	2.8
2	H	450	LYS	2.8
2	B	460	LEU	2.8
2	B	477	LYS	2.8
2	D	343	PHE	2.8
2	F	488	ASN	2.8
1	C	7	ILE	2.8
2	F	354	GLY	2.8
2	F	497	SER	2.8
2	H	376	GLN	2.8
2	B	348	TRP	2.8
2	B	486	ILE	2.8
1	E	20	VAL	2.7
1	A	321	LEU	2.7
1	G	5	ASP	2.7
2	H	479	ASP	2.7
2	H	477	LYS	2.7
2	F	351	MET	2.7
2	H	459	GLN	2.7
2	D	357	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	317	LEU	2.6
2	F	373	GLU	2.6
1	C	314	ARG	2.6
1	G	317	LEU	2.6
1	G	23	ILE	2.6
1	G	318	ALA	2.6
2	D	466	GLU	2.6
2	H	476	HIS	2.6
2	H	462	ASP	2.6
2	D	382	VAL	2.5
2	H	432	LEU	2.5
2	F	469	ASN	2.5
2	B	357	GLY	2.5
2	F	477	LYS	2.5
1	E	23	ILE	2.5
2	H	375	THR	2.5
2	H	457	ARG	2.5
2	H	351	MET	2.5
2	H	345	GLU	2.4
2	B	488	ASN	2.4
2	H	483	MET	2.4
2	D	350	GLY	2.4
2	F	470	GLY	2.4
1	E	321	LEU	2.4
2	F	340	ILE	2.4
2	H	452	LEU	2.4
2	F	486	ILE	2.4
1	E	11	TYR	2.4
2	D	352	VAL	2.4
2	F	440	ARG	2.4
1	A	36	ILE	2.4
2	D	474	PHE	2.3
1	C	6	GLN	2.3
2	B	482	CYS	2.3
2	H	461	ARG	2.3
2	B	466	GLU	2.3
2	D	354	GLY	2.3
2	F	442	LEU	2.3
2	F	370	ALA	2.3
2	B	354	GLY	2.3
2	F	459	GLN	2.3
2	H	478	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	370	ALA	2.2
2	D	358	TYR	2.2
1	E	324	SER	2.2
1	G	321	LEU	2.2
2	D	355	TRP	2.2
2	B	490	THR	2.2
1	E	36	ILE	2.2
2	H	377	LYS	2.2
1	A	18	GLU	2.2
2	F	441	THR	2.2
2	B	358	TYR	2.2
1	E	314	ARG	2.2
1	G	32	HIS	2.2
1	A	15	ASN	2.1
1	G	34	GLN	2.1
2	B	472	PHE	2.1
2	F	379	ILE	2.1
2	D	490	THR	2.1
2	F	383	THR	2.1
2	D	359	HIS	2.1
2	H	340	ILE	2.0
2	F	457	ARG	2.0
2	B	451	ASN	2.0
1	A	324	SER	2.0
2	F	367	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SIA	E	602	20/21	0.96	0.16	-0.68	31,47,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SIA	C	602	20/21	0.97	0.14	-1.16	26,46,56,58	0
4	SIA	A	602	20/21	0.97	0.14	-1.42	30,43,49,53	0
5	SIA	G	602	20/21	0.97	0.13	-2.15	35,47,57,60	0
4	GAL	A	603	12/12	0.82	0.24	-	87,101,125,135	0
5	NAG	G	604	15/15	0.82	0.19	-	95,118,133,134	0
5	NAG	E	604	15/15	0.78	0.23	-	110,121,137,139	0
4	GAL	C	603	12/12	0.86	0.17	-	71,111,126,129	0
5	GAL	E	603	11/12	0.87	0.19	-	61,88,126,129	0
5	GAL	G	603	11/12	0.90	0.16	-	60,92,113,123	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	G	601	14/15	0.90	0.16	0.25	40,68,80,82	0
3	NAG	E	601	14/15	0.90	0.16	-0.31	44,68,84,85	0
3	NAG	C	601	14/15	0.91	0.15	-0.39	50,64,83,96	0
3	NAG	A	601	14/15	0.91	0.15	-0.56	49,75,89,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.