



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:03 AM GMT

PDB ID : 1HGG  
Title : BINDING OF INFLUENZA VIRUS HEMAGGLUTININ TO ANALOGS OF ITS CELL-SURFACE RECEPTOR, SIALIC ACID: ANALYSIS BY PROTON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY AND X-RAY CRYSTALLOGRAPHY  
Authors : Sauter, N.K.; Hanson, J.E.; Glick, G.D.; Brown, J.H.; Crowther, R.L.; Park, S.-J.; Skehel, J.J.; Wiley, D.C.  
Deposited on : 1991-11-01  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

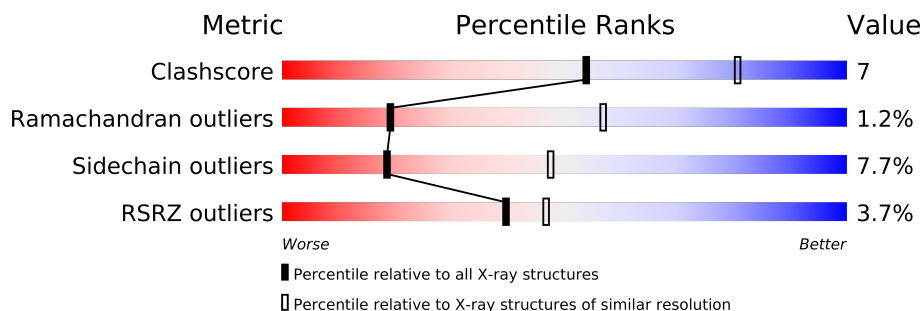
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	328	
1	C	328	
1	E	328	
2	B	175	
2	D	175	
2	F	175	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	329	-	X
3	NAG	A	334	-	X
3	NAG	A	348	-	X
3	NAG	B	401	-	X
3	NAG	C	329	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	C	348	-	X
3	NAG	D	401	-	X
3	NAG	E	329	-	X
3	NAG	E	348	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15882 atoms, of which 3408 are hydrogens and 0 are deuterium.

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, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3120	1581	588	445	493	13			

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	D	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			
2	F	175	Total	C	H	N	O	S	0	0	0
			1752	882	331	250	283	6			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	F	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
4	C	3	Total	C	H	N	O	0	0
			76	22	37	2	15		
4	E	3	Total	C	H	N	O	0	0
			76	22	37	2	15		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	3	Total	C	H	N	O	0	0
			81	23	38	1	19		
5	A	3	Total	C	H	N	O	0	0
			81	23	38	1	19		
5	C	3	Total	C	H	N	O	0	0
			81	23	38	1	19		
5	C	3	Total	C	H	N	O	0	0
			81	23	38	1	19		
5	E	3	Total	C	H	N	O	0	0
			81	23	38	1	19		
5	E	3	Total	C	H	N	O	0	0
			81	23	38	1	19		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	13	Total	H	O	0	0
			39	26	13		
6	B	11	Total	H	O	0	0
			33	22	11		
6	C	11	Total	H	O	0	0
			33	22	11		
6	D	13	Total	H	O	0	0
			39	26	13		
6	E	12	Total	H	O	0	0
			36	24	12		
6	F	12	Total	H	O	0	0
			36	24	12		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

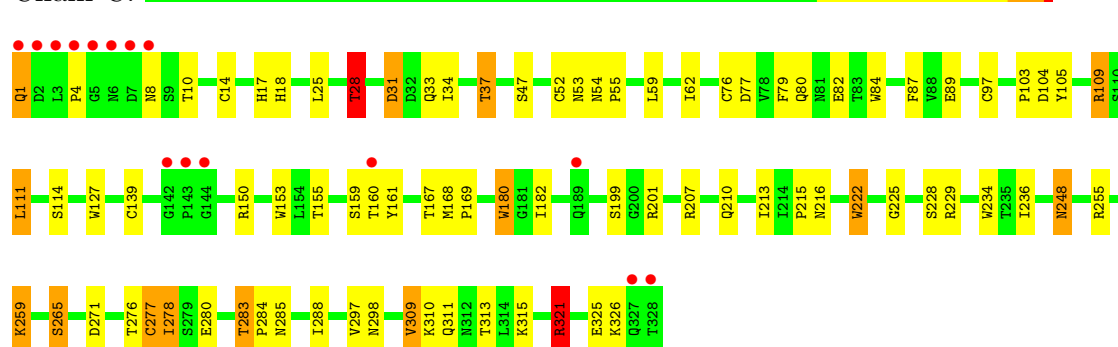
#### • Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain A:



#### • Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain C:



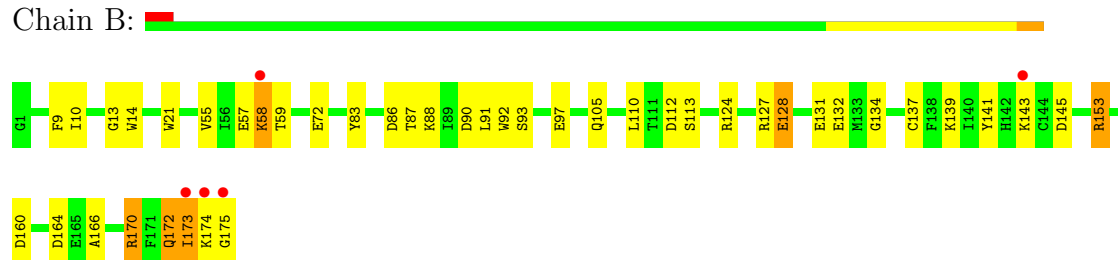
#### • Molecule 1: HEMAGGLUTININ, CHAIN HA1

Chain E:



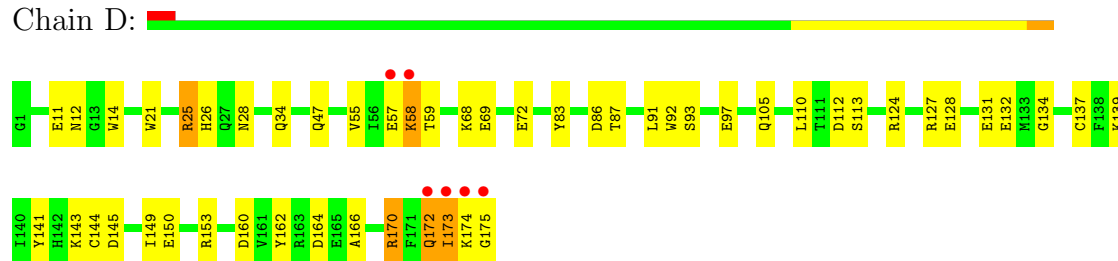
- Molecule 2: HEMAGGLUTININ, CHAIN HA2

Chain B:



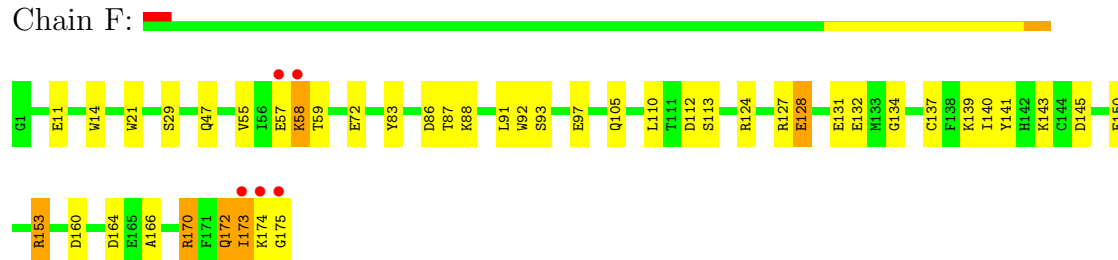
- Molecule 2: HEMAGGLUTININ, CHAIN HA2

Chain D:



- Molecule 2: HEMAGGLUTININ, CHAIN HA2

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.70Å 162.70Å 177.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.90 18.81 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.90) 69.2 (18.81-2.91)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.93Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.229 , (Not available) 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.6	EDS
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 69831 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	15882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, BGC, BMA, 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	0.91	2/2589 (0.1%)	1.47	38/3527 (1.1%)
1	C	0.89	1/2589 (0.0%)	1.45	33/3527 (0.9%)
1	E	0.92	1/2589 (0.0%)	1.48	36/3527 (1.0%)
2	B	0.92	0/1445	1.46	15/1939 (0.8%)
2	D	0.96	0/1445	1.49	20/1939 (1.0%)
2	F	0.95	0/1445	1.46	15/1939 (0.8%)
All	All	0.92	4/12102 (0.0%)	1.47	157/16398 (1.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	234	TRP	CG-CD2	-5.97	1.33	1.43
1	A	310	LYS	CD-CE	5.47	1.65	1.51
1	C	310	LYS	CD-CE	5.24	1.64	1.51
1	A	234	TRP	CG-CD2	-5.05	1.35	1.43

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	A	321	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	C	321	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	E	321	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	C	321	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	321	ARG	NE-CZ-NH1	9.93	125.27	120.30
2	D	153	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	D	14	TRP	CD1-CG-CD2	8.96	113.47	106.30
1	E	180	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	C	180	TRP	CD1-CG-CD2	8.66	113.23	106.30
2	B	14	TRP	CD1-CG-CD2	8.66	113.23	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	92	TRP	CD1-CG-CD2	8.60	113.18	106.30
1	E	105	TYR	CB-CG-CD2	-8.58	115.86	121.00
1	A	180	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	A	222	TRP	CD1-CG-CD2	8.30	112.94	106.30
2	F	14	TRP	CD1-CG-CD2	8.21	112.86	106.30
1	E	84	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	E	222	TRP	CD1-CG-CD2	8.13	112.80	106.30
2	F	124	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	B	92	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	105	TYR	CB-CG-CD2	-7.99	116.21	121.00
2	B	124	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	A	127	TRP	CD1-CG-CD2	7.92	112.63	106.30
2	F	21	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	C	222	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	C	105	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	E	207	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	E	326	LYS	CA-CB-CG	7.72	130.38	113.40
1	C	180	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	E	255	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	A	180	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	E	84	TRP	CE2-CD2-CG	-7.49	101.31	107.30
2	B	57	GLU	CA-CB-CG	7.48	129.87	113.40
1	C	255	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	D	14	TRP	CE2-CD2-CG	-7.46	101.33	107.30
2	F	57	GLU	CA-CB-CG	7.46	129.81	113.40
1	E	180	TRP	CE2-CD2-CG	-7.44	101.34	107.30
2	D	57	GLU	CA-CB-CG	7.41	129.71	113.40
1	C	127	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	E	222	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	A	1	GLN	N-CA-C	-7.29	91.32	111.00
2	F	153	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	D	21	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	234	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	C	84	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	A	127	TRP	CE2-CD2-CG	-7.24	101.50	107.30
1	E	104	ASP	CB-CG-OD1	7.22	124.80	118.30
1	C	255	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	D	92	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	B	92	TRP	CE2-CD2-CG	-7.13	101.59	107.30
2	F	92	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	C	127	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	E	127	TRP	CD1-CG-CD2	7.06	111.95	106.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	A	222	TRP	CE2-CD2-CG	-7.00	101.70	107.30
2	B	14	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	C	207	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	B	21	TRP	CD1-CG-CD2	6.92	111.83	106.30
1	A	255	ARG	NE-CZ-NH1	6.91	123.76	120.30
2	F	21	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	E	28	THR	CA-CB-CG2	6.87	122.02	112.40
1	A	84	TRP	CD1-CG-CD2	6.85	111.78	106.30
2	B	153	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	84	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	A	84	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	C	153	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	C	234	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	E	109	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	153	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	E	255	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	E	127	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	E	234	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	C	161	TYR	CB-CG-CD2	-6.61	117.03	121.00
1	A	207	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	E	180	TRP	CG-CD2-CE3	6.59	139.83	133.90
1	A	234	TRP	CE2-CD2-CG	-6.58	102.03	107.30
2	F	92	TRP	CE2-CD2-CG	-6.58	102.03	107.30
2	F	14	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	C	28	THR	CA-CB-CG2	6.53	121.54	112.40
2	B	21	TRP	CE2-CD2-CG	-6.52	102.09	107.30
1	C	104	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	28	THR	CA-CB-CG2	6.41	121.37	112.40
2	B	90	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	255	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	C	153	TRP	CE2-CD2-CG	-6.31	102.25	107.30
2	D	25	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	234	TRP	CE2-CD2-CG	-6.26	102.29	107.30
1	C	248	ASN	N-CA-CB	-6.24	99.38	110.60
1	C	234	TRP	CE2-CD2-CG	-6.19	102.35	107.30
1	A	104	ASP	CB-CG-OD1	6.18	123.86	118.30
2	D	112	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	159	SER	N-CA-CB	-6.17	101.25	110.50
2	D	14	TRP	CG-CD1-NE1	-6.11	104.00	110.10
2	D	124	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	248	ASN	N-CA-CB	-6.07	99.67	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	PRO	O-C-N	6.06	132.39	122.70
2	D	21	TRP	CE2-CD2-CG	-6.05	102.46	107.30
1	E	153	TRP	CD1-CG-CD2	6.04	111.13	106.30
1	E	1	GLN	N-CA-C	-6.03	94.73	111.00
1	C	1	GLN	N-CA-C	-6.02	94.76	111.00
1	A	180	TRP	CG-CD2-CE3	5.94	139.24	133.90
1	C	180	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	E	229	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	C	109	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	E	180	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	E	73	ASP	CB-CG-OD1	5.84	123.55	118.30
1	E	248	ASN	N-CA-CB	-5.83	100.10	110.60
1	A	109	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	C	180	TRP	CG-CD2-CE3	5.82	139.14	133.90
2	D	11	GLU	CA-CB-CG	-5.81	100.61	113.40
1	C	229	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	201	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	B	14	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	A	325	GLU	CA-CB-CG	5.71	125.97	113.40
2	B	112	ASP	CB-CG-OD1	5.71	123.44	118.30
2	B	86	ASP	CB-CG-OD1	5.64	123.37	118.30
1	E	153	TRP	CE2-CD2-CG	-5.61	102.81	107.30
2	D	55	VAL	CG1-CB-CG2	-5.61	101.93	110.90
2	F	21	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	A	321	ARG	CB-CG-CD	-5.61	97.03	111.60
1	E	229	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	E	76	CYS	CA-CB-SG	-5.58	103.95	114.00
2	F	170	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	D	25	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	321	ARG	CB-CG-CD	-5.54	97.20	111.60
1	A	180	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	A	271	ASP	CB-CG-OD1	5.50	123.25	118.30
2	F	14	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	C	180	TRP	CB-CG-CD1	-5.47	119.89	127.00
1	A	153	TRP	CE2-CD2-CG	-5.46	102.93	107.30
1	A	201	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	E	321	ARG	CB-CG-CD	-5.38	97.61	111.60
1	C	76	CYS	CA-CB-SG	-5.38	104.32	114.00
1	E	37	THR	CA-CB-CG2	5.36	119.90	112.40
2	D	21	TRP	CG-CD1-NE1	-5.34	104.76	110.10
2	B	55	VAL	CG1-CB-CG2	-5.33	102.37	110.90
1	E	180	TRP	CB-CG-CD1	-5.29	120.13	127.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	ASP	CB-CG-OD1	5.26	123.03	118.30
2	F	112	ASP	CB-CG-OD1	5.25	123.03	118.30
2	F	55	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	127	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	E	84	TRP	CG-CD2-CE3	5.24	138.62	133.90
2	D	162	TYR	CB-CG-CD1	-5.22	117.86	121.00
1	C	229	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	D	92	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	C	201	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	B	21	TRP	CG-CD1-NE1	-5.15	104.95	110.10
1	A	326	LYS	N-CA-C	-5.13	97.15	111.00
1	A	222	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	E	161	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	F	86	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	161	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	68	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	180	TRP	CB-CG-CD1	-5.04	120.45	127.00
1	A	153	TRP	CG-CD1-NE1	-5.02	105.08	110.10
2	D	86	ASP	CB-CG-OD1	5.02	122.82	118.30
2	D	170	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	588	1889	38	0
1	C	2532	588	1889	40	0
1	E	2532	588	1889	40	0
2	B	1421	331	1015	26	0
2	D	1421	331	1015	28	0
2	F	1421	331	1015	28	0
3	A	42	42	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	14	0	0	0
3	C	42	42	0	0	0
3	D	14	14	0	0	0
3	E	42	42	0	0	0
3	F	14	14	0	0	0
4	A	39	37	0	1	0
4	C	39	37	0	2	0
4	E	39	37	0	1	0
5	A	86	76	0	1	0
5	C	86	76	0	1	0
5	E	86	76	0	1	0
6	A	13	26	0	1	0
6	B	11	22	0	1	0
6	C	11	22	0	2	0
6	D	13	26	0	1	0
6	E	12	24	0	3	0
6	F	12	24	0	1	0
All	All	12474	3408	8712	169	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (169) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.48	0.79
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.49	0.77
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.46	0.77
2:B:83:TYR:O	2:B:87:THR:HG23	1.93	0.68
2:D:83:TYR:O	2:D:87:THR:HG23	1.95	0.67
2:F:83:TYR:O	2:F:87:THR:HG23	1.95	0.66
2:D:28:ASN:HB2	2:D:144:CYS:O	1.97	0.64
1:E:321:ARG:HG2	1:E:321:ARG:NH1	2.16	0.61
1:E:52:CYS:HB3	1:E:277:CYS:O	2.02	0.60
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.17	0.60
2:F:87:THR:HG22	6:F:405:HOH:O	2.02	0.60
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.83	0.59
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.84	0.59
2:D:87:THR:HG22	6:D:404:HOH:O	2.02	0.59
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.83	0.59
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.83	0.59
1:A:52:CYS:HB3	1:A:277:CYS:O	2.03	0.58
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.19	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.69	0.58
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.86	0.58
1:C:52:CYS:HB3	1:C:277:CYS:O	2.03	0.58
2:B:141:TYR:O	2:B:166:ALA:HA	2.04	0.58
2:D:132:GLU:HG2	2:D:134:GLY:H	1.69	0.57
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.86	0.57
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.70	0.57
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.69	0.56
2:B:132:GLU:HG2	2:B:134:GLY:H	1.69	0.56
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.19	0.56
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.87	0.56
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.87	0.55
2:F:132:GLU:HG2	2:F:134:GLY:H	1.72	0.55
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.22	0.55
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.90	0.54
2:B:87:THR:HG22	6:B:404:HOH:O	2.08	0.53
2:D:141:TYR:O	2:D:166:ALA:HA	2.08	0.53
1:C:321:ARG:NH1	1:C:321:ARG:HG2	2.19	0.52
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.91	0.52
2:F:141:TYR:O	2:F:166:ALA:HA	2.10	0.52
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.46	0.51
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.46	0.51
1:A:25:LEU:HD13	1:A:33:GLN:HB3	1.93	0.51
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.93	0.50
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.46	0.50
1:E:25:LEU:HD13	1:E:33:GLN:HB3	1.94	0.49
1:C:309:VAL:HG22	2:D:93:SER:HA	1.94	0.49
1:A:309:VAL:HG22	2:B:93:SER:HA	1.94	0.49
1:A:77:ASP:O	1:A:80:GLN:HG3	2.13	0.49
1:A:28:THR:HG22	1:A:31:ASP:H	1.78	0.48
1:E:182:ILE:HD13	1:E:213:ILE:HG22	1.96	0.48
1:C:25:LEU:HD13	1:C:33:GLN:HB3	1.95	0.48
1:C:325:GLU:O	1:C:325:GLU:HG2	2.14	0.48
1:E:309:VAL:HG22	2:F:93:SER:HA	1.96	0.48
1:A:182:ILE:HD13	1:A:213:ILE:HG22	1.94	0.48
1:C:77:ASP:O	1:C:80:GLN:HG3	2.13	0.48
1:C:182:ILE:HD13	1:C:213:ILE:HG22	1.95	0.47
1:E:28:THR:HG22	1:E:31:ASP:H	1.78	0.47
1:C:114:SER:HA	1:C:265:SER:O	2.13	0.47
2:D:25:ARG:HG3	2:D:34:GLN:HG3	1.96	0.47
1:E:77:ASP:O	1:E:80:GLN:HG3	2.14	0.47
2:D:91:LEU:HD13	2:F:91:LEU:HD13	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:143:LYS:NZ	2:F:145:ASP:HB3	2.29	0.47
1:A:21:PRO:O	1:A:327:GLN:HG2	2.14	0.47
2:B:131:GLU:OE1	2:D:127:ARG:NH1	2.48	0.47
2:D:143:LYS:NZ	2:D:145:ASP:HB3	2.30	0.47
1:C:10:THR:HG21	2:D:139:LYS:HE2	1.97	0.47
1:C:28:THR:HG23	2:D:105:GLN:OE1	2.13	0.47
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.46
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.97	0.46
1:C:28:THR:HG22	1:C:31:ASP:H	1.81	0.46
1:C:53:ASN:OD1	1:C:276:THR:HA	2.14	0.46
1:E:47:SER:HA	1:E:288:ILE:HG22	1.96	0.46
1:C:79:PHE:O	1:C:82:GLU:HB2	2.16	0.46
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.49	0.46
1:E:10:THR:HG21	2:F:139:LYS:HE2	1.97	0.46
1:A:47:SER:HA	1:A:288:ILE:HG22	1.96	0.46
1:A:59:LEU:HD23	1:A:87:PHE:CD2	2.51	0.45
1:A:284:PRO:HG2	1:A:298:ASN:ND2	2.30	0.45
1:C:284:PRO:HG2	1:C:298:ASN:ND2	2.31	0.45
1:C:47:SER:HA	1:C:288:ILE:HG22	1.98	0.45
1:A:10:THR:HG21	2:B:139:LYS:HE2	1.98	0.45
1:C:59:LEU:HD23	1:C:87:PHE:CD2	2.51	0.45
1:E:167:THR:HB	4:E:339:NAG:H62	1.99	0.45
1:A:97:CYS:HA	1:A:139:CYS:HA	1.98	0.45
1:C:97:CYS:HA	1:C:139:CYS:HA	1.98	0.45
1:A:167:THR:HB	4:A:339:NAG:H62	1.99	0.45
2:B:58:LYS:HE2	2:B:59:THR:O	2.17	0.45
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.32	0.45
1:E:114:SER:HA	1:E:265:SER:O	2.17	0.44
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.17	0.44
1:C:167:THR:HB	4:C:339:NAG:H62	2.00	0.44
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.33	0.44
2:F:110:LEU:O	2:F:113:SER:HB3	2.17	0.44
1:A:114:SER:HA	1:A:265:SER:O	2.18	0.44
1:C:37:THR:HG21	6:C:357:HOH:O	2.18	0.44
1:E:180:TRP:CH2	1:E:213:ILE:HD13	2.52	0.44
2:D:47:GLN:HB3	2:D:110:LEU:HD11	2.00	0.44
1:E:79:PHE:O	1:E:82:GLU:HB2	2.17	0.44
2:D:58:LYS:HE2	2:D:59:THR:O	2.18	0.44
5:A:354:SIA:H32	2:B:72:GLU:HG2	2.00	0.44
1:A:28:THR:HG23	2:B:105:GLN:OE1	2.18	0.43
2:B:143:LYS:NZ	2:B:145:ASP:HB3	2.33	0.43
2:F:58:LYS:HE2	2:F:59:THR:O	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:141:ARG:NH1	1:E:147:PHE:O	2.48	0.43
1:C:283:THR:HG22	1:C:285:ASN:H	1.83	0.43
5:C:354:SIA:H32	2:D:72:GLU:HG2	2.00	0.43
1:E:17:HIS:CE1	6:E:363:HOH:H1	2.35	0.43
1:A:14:CYS:HA	2:B:137:CYS:HA	2.00	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.00	0.43
2:B:88:LYS:HD2	2:F:87:THR:HG21	1.99	0.43
2:B:127:ARG:HB3	2:B:128:GLU:H	1.68	0.43
2:B:110:LEU:O	2:B:113:SER:HB3	2.19	0.43
2:B:58:LYS:HG3	2:B:59:THR:O	2.18	0.43
1:C:89:GLU:OE1	1:C:109:ARG:NH1	2.51	0.43
1:E:59:LEU:HD23	1:E:87:PHE:CD2	2.53	0.43
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.52	0.43
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.18	0.43
1:C:180:TRP:CH2	1:C:213:ILE:HD13	2.51	0.43
1:C:53:ASN:HD21	1:C:276:THR:HG23	1.83	0.43
1:E:97:CYS:HA	1:E:139:CYS:HA	1.99	0.43
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.52	0.43
1:E:283:THR:HG22	1:E:285:ASN:H	1.83	0.43
2:F:127:ARG:HB3	2:F:128:GLU:H	1.66	0.42
1:C:313:THR:OG1	1:C:315:LYS:NZ	2.52	0.42
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.34	0.42
1:A:221:PRO:HA	4:C:340:NAG:O7	2.18	0.42
1:E:313:THR:OG1	1:E:315:LYS:NZ	2.53	0.42
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.55	0.42
2:B:128:GLU:HG3	2:B:170:ARG:HH21	1.85	0.42
2:F:47:GLN:HB3	2:F:110:LEU:HD11	2.01	0.42
1:C:17:HIS:CE1	6:C:362:HOH:H1	2.36	0.42
1:E:109:ARG:HD2	1:E:109:ARG:HH11	1.66	0.42
2:D:58:LYS:HG3	2:D:59:THR:O	2.20	0.42
1:E:37:THR:HG21	6:E:357:HOH:O	2.18	0.42
2:D:131:GLU:OE1	2:F:127:ARG:NH1	2.52	0.42
1:A:37:THR:HG21	6:A:357:HOH:O	2.19	0.42
2:D:68:LYS:O	2:D:69:GLU:HG3	2.20	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
2:D:26:HIS:CD2	2:D:149:ILE:HG13	2.55	0.41
1:A:75:HIS:HE1	1:A:94:PHE:O	2.04	0.41
2:F:58:LYS:HG3	2:F:59:THR:O	2.20	0.41
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.53	0.41
1:A:141:ARG:NH1	1:A:147:PHE:O	2.49	0.41
5:E:354:SIA:H32	2:F:72:GLU:HG2	2.01	0.41
1:A:66:LEU:HD22	1:A:267:ILE:HD12	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:182:ILE:HD11	1:E:215:PRO:HD3	2.02	0.41
1:A:10:THR:HG22	2:B:141:TYR:HA	2.03	0.41
1:C:182:ILE:HD11	1:C:215:PRO:HD3	2.03	0.41
1:E:10:THR:HG22	2:F:141:TYR:HA	2.02	0.41
1:C:325:GLU:HB2	2:D:12:ASN:ND2	2.35	0.41
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.64	0.41
2:D:26:HIS:CE1	2:D:149:ILE:HG21	2.55	0.41
1:A:75:HIS:CE1	1:A:94:PHE:O	2.74	0.41
1:C:259:LYS:HB2	1:C:259:LYS:NZ	2.35	0.41
1:A:139:CYS:HB3	1:A:146:GLY:O	2.21	0.41
1:C:283:THR:HG22	1:C:285:ASN:N	2.35	0.41
1:E:139:CYS:HB3	1:E:146:GLY:O	2.21	0.41
1:E:283:THR:HG22	1:E:285:ASN:N	2.36	0.41
1:E:37:THR:HG21	6:E:357:HOH:H2	1.85	0.41
1:A:325:GLU:HB2	2:B:13:GLY:O	2.21	0.41
1:A:202:VAL:O	1:A:212:THR:HA	2.22	0.40
1:E:11:ALA:HB3	2:F:140:ILE:HB	2.03	0.40
1:C:168:MET:HA	1:C:169:PRO:HD3	1.88	0.40
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.22	0.40
1:C:288:ILE:HG21	1:C:297:VAL:HG21	2.03	0.40
1:C:111:LEU:HD21	1:C:236:ILE:HD11	2.03	0.40
1:A:168:MET:HA	1:A:169:PRO:HD3	1.87	0.40
2:D:110:LEU:O	2:D:113:SER:HB3	2.22	0.40
1:E:203:THR:HA	1:E:211:GLN:O	2.21	0.40
1:A:283:THR:HG22	1:A:285:ASN:H	1.86	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	326/328 (99%)	304 (93%)	17 (5%)	5 (2%)	15	50	
1	C	326/328 (99%)	307 (94%)	16 (5%)	3 (1%)	25	66	
1	E	326/328 (99%)	309 (95%)	16 (5%)	1 (0%)	50	85	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	45
2	D	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	45
2	F	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	45
All	All	1497/1509 (99%)	1400 (94%)	79 (5%)	18 (1%)	19	57

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	326	LYS
2	B	58	LYS
2	B	173	ILE
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	327	GLN
1	C	326	LYS
2	B	172	GLN
2	D	172	GLN
2	F	172	GLN
1	A	2	ASP
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	C	4	PRO

### 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	289/289 (100%)	259 (90%)	30 (10%)	10	29
1	C	289/289 (100%)	264 (91%)	25 (9%)	15	41
1	E	289/289 (100%)	259 (90%)	30 (10%)	10	29
2	B	149/149 (100%)	144 (97%)	5 (3%)	49	86

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	149/149 (100%)	144 (97%)	5 (3%)	49	86
2	F	149/149 (100%)	143 (96%)	6 (4%)	42	81
All	All	1314/1314 (100%)	1213 (92%)	101 (8%)	18	47

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	8	ASN
1	A	18	HIS
1	A	28	THR
1	A	31	ASP
1	A	34	ILE
1	A	37	THR
1	A	54	ASN
1	A	82	GLU
1	A	103	PRO
1	A	111	LEU
1	A	150	ARG
1	A	155	THR
1	A	156	LYS
1	A	157	SER
1	A	160	THR
1	A	199	SER
1	A	210	GLN
1	A	228	SER
1	A	248	ASN
1	A	259	LYS
1	A	265	SER
1	A	277	CYS
1	A	278	ILE
1	A	280	GLU
1	A	283	THR
1	A	299	LYS
1	A	309	VAL
1	A	321	ARG
1	A	326	LYS
2	B	128	GLU
2	B	153	ARG
2	B	160	ASP
2	B	170	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	172	GLN
1	C	8	ASN
1	C	18	HIS
1	C	28	THR
1	C	31	ASP
1	C	34	ILE
1	C	37	THR
1	C	54	ASN
1	C	103	PRO
1	C	111	LEU
1	C	150	ARG
1	C	155	THR
1	C	159	SER
1	C	160	THR
1	C	199	SER
1	C	210	GLN
1	C	228	SER
1	C	248	ASN
1	C	259	LYS
1	C	265	SER
1	C	277	CYS
1	C	278	ILE
1	C	280	GLU
1	C	283	THR
1	C	309	VAL
1	C	321	ARG
2	D	128	GLU
2	D	150	GLU
2	D	160	ASP
2	D	170	ARG
2	D	172	GLN
1	E	2	ASP
1	E	8	ASN
1	E	18	HIS
1	E	28	THR
1	E	31	ASP
1	E	34	ILE
1	E	37	THR
1	E	54	ASN
1	E	82	GLU
1	E	103	PRO
1	E	111	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	150	ARG
1	E	155	THR
1	E	159	SER
1	E	160	THR
1	E	189	GLN
1	E	199	SER
1	E	210	GLN
1	E	228	SER
1	E	248	ASN
1	E	259	LYS
1	E	265	SER
1	E	277	CYS
1	E	278	ILE
1	E	280	GLU
1	E	283	THR
1	E	309	VAL
1	E	321	ARG
1	E	326	LYS
1	E	328	THR
2	F	11	GLU
2	F	29	SER
2	F	128	GLU
2	F	160	ASP
2	F	170	ARG
2	F	172	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	81	ASN
1	A	132	GLN
1	A	171	ASN
2	B	28	ASN
2	B	49	ASN
2	B	146	ASN
1	C	38	ASN
1	C	81	ASN
1	C	132	GLN
1	C	171	ASN
2	D	12	ASN
1	E	8	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	38	ASN
1	E	81	ASN
1	E	132	GLN
1	E	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

27 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	NAG	A	339	1,4	12,14,15	0.61	0	15,19,21	0.99	1 (6%)
4	NAG	A	340	4	12,14,15	0.80	0	15,19,21	1.10	2 (13%)
4	BMA	A	341	4	10,11,12	0.54	0	11,15,17	0.80	0
5	GAL	A	349	5	10,11,12	0.71	0	11,15,17	1.04	1 (9%)
5	BGC	A	350	5	12,12,12	1.27	1 (8%)	17,17,17	1.04	2 (11%)
5	SIA	A	351	5	20,20,21	3.93	2 (10%)	23,28,31	2.98	6 (26%)
5	GAL	A	352	5	10,11,12	0.76	0	11,15,17	0.98	1 (9%)
5	BGC	A	353	5	12,12,12	0.55	0	17,17,17	0.89	0
5	SIA	A	354	5	20,20,21	3.83	3 (15%)	23,28,31	3.19	5 (21%)
4	NAG	C	339	1,4	12,14,15	0.69	0	15,19,21	1.05	1 (6%)
4	NAG	C	340	4	12,14,15	0.52	0	15,19,21	1.12	3 (20%)
4	BMA	C	341	4	10,11,12	0.62	0	11,15,17	1.04	1 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GAL	C	349	5	10,11,12	0.82	0	11,15,17	1.07	1 (9%)
5	BGC	C	350	5	12,12,12	1.28	1 (8%)	17,17,17	0.96	1 (5%)
5	SIA	C	351	5	20,20,21	3.75	3 (15%)	23,28,31	2.87	4 (17%)
5	GAL	C	352	5	10,11,12	0.77	0	11,15,17	0.95	1 (9%)
5	BGC	C	353	5	12,12,12	0.57	0	17,17,17	0.79	0
5	SIA	C	354	5	20,20,21	3.95	3 (15%)	23,28,31	3.15	5 (21%)
4	NAG	E	339	1,4	12,14,15	0.82	0	15,19,21	0.97	1 (6%)
4	NAG	E	340	4	12,14,15	0.63	0	15,19,21	1.06	2 (13%)
4	BMA	E	341	4	10,11,12	0.82	0	11,15,17	1.98	2 (18%)
5	GAL	E	349	5	10,11,12	0.76	0	11,15,17	1.08	0
5	BGC	E	350	5	12,12,12	1.15	1 (8%)	17,17,17	1.02	1 (5%)
5	SIA	E	351	5	20,20,21	3.56	2 (10%)	23,28,31	2.96	5 (21%)
5	GAL	E	352	5	10,11,12	0.81	0	11,15,17	0.98	1 (9%)
5	BGC	E	353	5	12,12,12	0.47	0	17,17,17	0.76	0
5	SIA	E	354	5	20,20,21	4.00	3 (15%)	23,28,31	3.13	6 (26%)

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	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	340	4	-	0/6/23/26	0/1/1/1
4	BMA	A	341	4	-	0/2/19/22	0/1/1/1
5	GAL	A	349	5	-	0/2/19/22	0/1/1/1
5	BGC	A	350	5	-	0/2/22/22	0/1/1/1
5	SIA	A	351	5	-	0/15/34/38	0/1/1/1
5	GAL	A	352	5	-	0/2/19/22	0/1/1/1
5	BGC	A	353	5	-	0/2/22/22	0/1/1/1
5	SIA	A	354	5	-	0/15/34/38	0/1/1/1
4	NAG	C	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	340	4	-	0/6/23/26	0/1/1/1
4	BMA	C	341	4	-	0/2/19/22	0/1/1/1
5	GAL	C	349	5	-	0/2/19/22	0/1/1/1
5	BGC	C	350	5	-	0/2/22/22	0/1/1/1
5	SIA	C	351	5	-	0/15/34/38	0/1/1/1
5	GAL	C	352	5	-	0/2/19/22	0/1/1/1
5	BGC	C	353	5	-	0/2/22/22	0/1/1/1
5	SIA	C	354	5	-	0/15/34/38	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	339	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	340	4	-	0/6/23/26	0/1/1/1
4	BMA	E	341	4	-	0/2/19/22	0/1/1/1
5	GAL	E	349	5	-	0/2/19/22	0/1/1/1
5	BGC	E	350	5	-	0/2/22/22	0/1/1/1
5	SIA	E	351	5	-	0/15/34/38	0/1/1/1
5	GAL	E	352	5	-	0/2/19/22	0/1/1/1
5	BGC	E	353	5	-	0/2/22/22	0/1/1/1
5	SIA	E	354	5	-	0/15/34/38	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	354	SIA	O6-C2	17.37	1.44	1.28
5	C	354	SIA	O6-C2	17.18	1.44	1.28
5	A	351	SIA	O6-C2	17.02	1.43	1.28
5	A	354	SIA	O6-C2	16.68	1.43	1.28
5	C	351	SIA	O6-C2	16.14	1.43	1.28
5	E	351	SIA	O6-C2	15.31	1.42	1.28
5	A	350	BGC	C4-C5	2.96	1.59	1.53
5	C	350	BGC	C4-C5	2.86	1.59	1.53
5	E	350	BGC	C4-C5	2.71	1.59	1.53
5	C	351	SIA	O1B-C1	-2.43	1.22	1.30
5	E	351	SIA	O1B-C1	-2.38	1.22	1.30
5	A	351	SIA	O1B-C1	-2.36	1.22	1.30
5	C	354	SIA	C3-C2	2.19	1.54	1.46
5	A	354	SIA	C3-C2	2.07	1.53	1.46
5	C	351	SIA	C3-C2	2.06	1.53	1.46
5	E	354	SIA	C3-C2	2.05	1.53	1.46
5	A	354	SIA	O1B-C1	-2.03	1.24	1.30
5	E	354	SIA	O1B-C1	-2.01	1.24	1.30
5	C	354	SIA	O1B-C1	-2.00	1.24	1.30

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	354	SIA	O6-C2-C3	-13.96	106.67	124.91
5	C	354	SIA	O6-C2-C3	-13.77	106.92	124.91
5	E	354	SIA	O6-C2-C3	-13.43	107.37	124.91
5	A	351	SIA	O6-C2-C3	-12.84	108.13	124.91
5	E	351	SIA	O6-C2-C3	-12.79	108.20	124.91
5	C	351	SIA	O6-C2-C3	-12.41	108.69	124.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	341	BMA	O5-C5-C6	4.88	112.10	106.98
4	E	341	BMA	O5-C5-C4	-3.69	105.97	110.65
4	C	339	NAG	C3-C2-N2	-3.33	106.70	111.76
4	A	339	NAG	C3-C2-N2	-3.20	106.88	111.76
4	E	339	NAG	C3-C2-N2	-3.00	107.19	111.76
5	E	354	SIA	C7-C6-C5	2.82	118.40	114.24
5	E	352	GAL	C4-C3-C2	-2.75	106.82	110.50
5	E	354	SIA	O9-C9-C8	-2.67	105.07	111.05
5	A	352	GAL	C4-C3-C2	-2.62	106.99	110.50
4	C	341	BMA	C6-C5-C4	-2.61	106.69	113.00
5	C	354	SIA	C7-C6-C5	2.61	118.08	114.24
5	C	351	SIA	C4-C5-N5	-2.59	104.39	110.12
5	A	354	SIA	O9-C9-C8	-2.53	105.39	111.05
5	A	354	SIA	C7-C6-C5	2.52	117.96	114.24
5	C	352	GAL	C4-C3-C2	-2.48	107.18	110.50
5	E	354	SIA	C11-C10-N5	2.44	120.88	116.11
5	C	351	SIA	C6-C5-N5	2.40	115.18	110.99
5	A	354	SIA	C11-C10-N5	2.36	120.73	116.11
5	C	354	SIA	O9-C9-C8	-2.35	105.80	111.05
5	A	350	BGC	C4-C3-C2	-2.34	106.49	110.82
5	A	351	SIA	C11-C10-N5	2.27	120.55	116.11
5	E	350	BGC	C4-C3-C2	-2.26	106.63	110.82
5	C	349	GAL	O5-C5-C4	-2.22	107.84	110.65
5	C	354	SIA	C11-C10-N5	2.21	120.43	116.11
5	E	351	SIA	C6-C5-N5	2.20	114.82	110.99
4	E	340	NAG	O5-C5-C4	-2.19	107.87	110.65
5	E	351	SIA	O9-C9-C8	-2.19	106.16	111.05
4	A	340	NAG	O5-C5-C4	-2.19	107.88	110.65
5	A	349	GAL	O5-C5-C4	-2.18	107.89	110.65
4	C	340	NAG	C3-C2-N2	-2.17	108.45	111.76
5	C	351	SIA	O4-C4-C3	2.17	114.07	109.08
5	E	351	SIA	C4-C5-N5	-2.14	105.39	110.12
5	A	351	SIA	C6-C5-N5	2.12	114.69	110.99
4	C	340	NAG	O5-C5-C4	-2.12	107.97	110.65
5	A	351	SIA	C4-C5-N5	-2.10	105.47	110.12
5	C	354	SIA	C8-C7-C6	-2.10	108.93	112.99
5	A	350	BGC	C1-O5-C5	2.09	117.15	113.40
4	C	340	NAG	O5-C5-C6	2.09	109.17	106.98
5	E	351	SIA	C11-C10-N5	2.08	120.17	116.11
5	A	351	SIA	O9-C9-C8	-2.07	106.43	111.05
4	A	340	NAG	C3-C2-N2	-2.04	108.65	111.76
5	A	351	SIA	O4-C4-C3	2.04	113.78	109.08

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	350	BGC	C4-C3-C2	-2.04	107.05	110.82
5	E	354	SIA	O10-C10-C11	-2.03	118.09	122.04
5	A	354	SIA	O10-C10-C11	-2.02	118.09	122.04
5	E	354	SIA	C8-C7-C6	-2.02	109.08	112.99
4	E	340	NAG	C3-C2-N2	-2.01	108.69	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

12 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	329	1	12,14,15	0.80	1 (8%)	15,19,21	1.01	0
3	NAG	A	334	1	12,14,15	0.61	0	15,19,21	1.55	2 (13%)
3	NAG	A	348	1	12,14,15	0.73	0	15,19,21	1.43	2 (13%)
3	NAG	B	401	2	12,14,15	0.83	0	15,19,21	1.07	1 (6%)
3	NAG	C	329	1	12,14,15	0.71	0	15,19,21	0.99	0
3	NAG	C	334	1	12,14,15	0.69	0	15,19,21	1.73	2 (13%)
3	NAG	C	348	1	12,14,15	0.69	0	15,19,21	1.53	3 (20%)
3	NAG	D	401	2	12,14,15	0.92	0	15,19,21	1.11	0
3	NAG	E	329	1	12,14,15	0.72	0	15,19,21	0.96	0
3	NAG	E	334	1	12,14,15	0.60	0	15,19,21	1.65	2 (13%)
3	NAG	E	348	1	12,14,15	0.69	0	15,19,21	1.49	4 (26%)
3	NAG	F	401	2	12,14,15	1.00	1 (8%)	15,19,21	1.03	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	329	1	-	0/6/23/26	0/1/1/1
3	NAG	A	334	1	-	0/6/23/26	0/1/1/1
3	NAG	A	348	1	-	0/6/23/26	0/1/1/1
3	NAG	B	401	2	-	0/6/23/26	0/1/1/1
3	NAG	C	329	1	-	0/6/23/26	0/1/1/1
3	NAG	C	334	1	-	0/6/23/26	0/1/1/1
3	NAG	C	348	1	-	0/6/23/26	0/1/1/1
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1
3	NAG	E	329	1	-	0/6/23/26	0/1/1/1
3	NAG	E	334	1	-	0/6/23/26	0/1/1/1
3	NAG	E	348	1	-	0/6/23/26	0/1/1/1
3	NAG	F	401	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	NAG	C4-C5	2.05	1.57	1.53
3	A	329	NAG	C4-C5	2.02	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	334	NAG	O5-C5-C6	4.30	111.50	106.98
3	E	334	NAG	O5-C5-C6	4.23	111.42	106.98
3	A	334	NAG	O5-C5-C6	3.78	110.95	106.98
3	C	334	NAG	O5-C5-C4	-3.55	106.15	110.65
3	E	334	NAG	O5-C5-C4	-3.33	106.42	110.65
3	A	334	NAG	O5-C5-C4	-3.08	106.74	110.65
3	C	348	NAG	O5-C5-C4	-2.99	106.86	110.65
3	A	348	NAG	O5-C5-C4	-2.75	107.16	110.65
3	E	348	NAG	C3-C4-C5	-2.51	105.73	110.20
3	E	348	NAG	O5-C5-C4	-2.47	107.52	110.65
3	E	348	NAG	C8-C7-N2	2.31	120.62	116.11
3	A	348	NAG	C3-C4-C5	-2.26	106.17	110.20
3	C	348	NAG	C3-C4-C5	-2.20	106.28	110.20
3	C	348	NAG	C8-C7-N2	2.19	120.39	116.11
3	B	401	NAG	C3-C2-N2	-2.16	108.47	111.76
3	E	348	NAG	O4-C4-C5	2.05	114.70	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	328/328 (100%)	-0.24	13 (3%) 36 43	6, 26, 52, 144	0
1	C	328/328 (100%)	-0.20	15 (4%) 31 38	6, 26, 51, 150	0
1	E	328/328 (100%)	-0.25	13 (3%) 36 43	6, 26, 52, 146	0
2	B	175/175 (100%)	-0.47	5 (2%) 49 58	3, 21, 51, 105	0
2	D	175/175 (100%)	-0.49	6 (3%) 43 51	3, 20, 50, 106	0
2	F	175/175 (100%)	-0.54	5 (2%) 49 58	2, 20, 50, 105	0
All	All	1509/1509 (100%)	-0.32	57 (3%) 39 45	2, 24, 52, 150	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	ASP	10.4
1	E	6	ASN	9.9
1	A	7	ASP	9.4
1	A	328	THR	9.1
1	C	7	ASP	8.2
1	C	3	LEU	7.6
1	E	1	GLN	7.5
1	A	327	GLN	7.5
1	C	8	ASN	7.4
1	A	4	PRO	7.4
1	A	3	LEU	7.3
1	C	5	GLY	7.3
1	C	4	PRO	7.3
1	C	6	ASN	6.9
1	A	8	ASN	6.8
1	E	328	THR	6.5
1	C	2	ASP	6.5
1	A	5	GLY	6.0
1	E	4	PRO	6.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	3	LEU	5.9
1	E	5	GLY	5.8
2	D	175	GLY	5.5
2	B	173	ILE	5.5
1	C	1	GLN	5.5
2	F	175	GLY	5.4
1	C	328	THR	5.4
2	D	173	ILE	5.3
2	F	173	ILE	5.1
2	B	175	GLY	5.1
1	A	2	ASP	5.0
1	A	6	ASN	4.9
2	F	174	LYS	4.8
1	E	2	ASP	4.8
1	A	326	LYS	4.0
2	D	57	GLU	3.9
1	E	327	GLN	3.9
2	B	58	LYS	3.4
2	D	58	LYS	3.3
1	E	8	ASN	3.2
2	B	174	LYS	3.2
1	A	1	GLN	3.1
1	A	143	PRO	3.0
2	D	174	LYS	3.0
1	E	142	GLY	2.9
2	F	58	LYS	2.6
1	C	143	PRO	2.5
1	C	142	GLY	2.4
1	E	9	SER	2.4
1	A	144	GLY	2.3
1	C	189	GLN	2.3
1	C	327	GLN	2.3
2	B	143	LYS	2.2
1	C	144	GLY	2.2
1	E	208	ARG	2.1
1	C	160	THR	2.0
2	F	57	GLU	2.0
2	D	172	GLN	2.0

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

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



### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	SIA	E	354	20/21	0.36	8.61	0,42,44,44	37
5	BGC	E	353	12/12	0.45	5.35	0,0,49,50	23
5	GAL	E	352	11/12	0.35	4.55	0,0,47,48	21
5	BGC	A	350	12/12	0.46	4.16	0,0,67,68	23
5	SIA	A	354	20/21	0.36	3.69	0,41,44,44	37
5	SIA	C	354	20/21	0.35	2.93	0,41,44,44	37
5	BGC	C	353	12/12	0.39	2.65	0,0,49,50	23
5	BGC	E	350	12/12	0.33	2.64	0,0,67,68	23
5	GAL	A	352	11/12	0.38	2.06	0,0,47,48	21
5	BGC	A	353	12/12	0.35	1.90	0,0,49,50	23
5	SIA	E	351	20/21	0.21	1.45	0,35,41,42	37
5	SIA	A	351	20/21	0.21	1.40	0,35,41,42	37
5	GAL	C	352	11/12	0.34	1.35	0,0,47,48	21
5	GAL	E	349	11/12	0.20	0.45	0,0,51,53	21
5	GAL	A	349	11/12	0.20	0.45	0,0,51,53	21
4	NAG	C	340	14/15	0.22	0.38	0,0,57,60	0
5	SIA	C	351	20/21	0.19	0.36	0,35,41,42	37
5	BGC	C	350	12/12	0.39	0.17	0,0,67,68	23
4	NAG	C	339	14/15	0.17	-0.04	0,0,45,48	0
4	NAG	A	340	14/15	0.16	-0.09	0,0,57,59	0
4	NAG	E	340	14/15	0.18	-0.32	0,0,57,59	0
5	GAL	C	349	11/12	0.16	-0.43	0,0,51,53	21
4	NAG	A	339	14/15	0.13	-0.50	0,0,45,48	0
4	NAG	E	339	14/15	0.13	-0.76	0,0,44,48	0
4	BMA	E	341	11/12	0.21	-	0,0,65,68	0
4	BMA	C	341	11/12	0.34	-	0,0,70,72	0
4	BMA	A	341	11/12	0.28	-	0,0,64,65	0

### 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. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	E	348	14/15	0.30	11.06	0,0,49,50	0
3	NAG	E	329	14/15	0.28	10.93	0,0,50,50	0
3	NAG	C	329	14/15	0.29	7.42	0,0,49,50	0
3	NAG	B	401	14/15	0.36	5.58	0,0,61,61	0
3	NAG	A	329	14/15	0.27	5.26	0,0,49,50	0
3	NAG	D	401	14/15	0.36	4.75	0,0,61,62	0
3	NAG	A	348	14/15	0.24	2.76	0,0,50,51	0
3	NAG	C	348	14/15	0.24	2.03	0,0,49,51	0
3	NAG	A	334	14/15	0.21	2.03	0,0,44,45	0
3	NAG	E	334	14/15	0.21	1.59	0,0,44,46	0
3	NAG	C	334	14/15	0.22	1.31	0,0,44,46	0
3	NAG	F	401	14/15	0.27	1.13	0,0,61,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.