



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID : 1HGD  
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 : 2.70 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

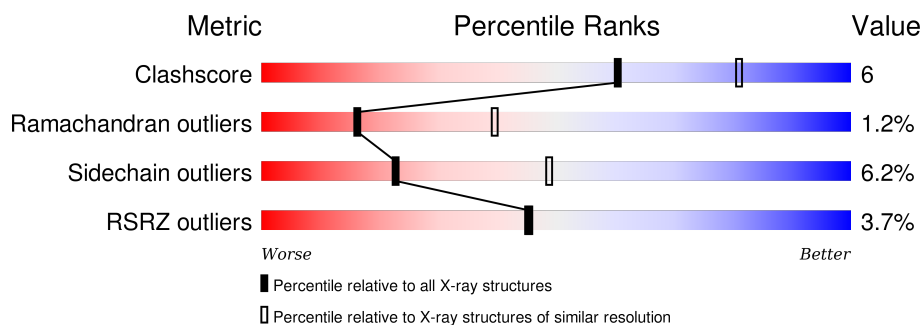
# 1 Overall quality at a glance

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))
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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	328	<div> <div>4%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	C	328	<div> <div>4%</div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
1	E	328	<div> <div>4%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
2	B	175	<div> <div>2%</div> <div>80%</div> <div>14%</div> <div>5% •</div> </div>
2	D	175	<div> <div>3%</div> <div>76%</div> <div>17%</div> <div>6% •</div> </div>
2	F	175	<div> <div>4%</div> <div>76%</div> <div>18%</div> <div>5% •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	329	-	-	-	X
3	NAG	A	348	-	-	-	X
3	NAG	B	401	-	-	-	X
3	NAG	C	329	-	-	-	X
3	NAG	C	334	-	-	-	X
3	NAG	C	348	-	-	-	X
3	NAG	D	401	-	-	-	X
3	NAG	E	329	-	-	-	X
3	NAG	E	334	-	-	-	X
3	NAG	E	348	-	-	-	X
3	NAG	F	401	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15432 atoms, of which 3195 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, CHAIN HA1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0	0
			3132	1585	593	448	493	13			
1	C	328	Total	C	H	N	O	S	0	0	0
			3132	1585	593	448	493	13			
1	E	328	Total	C	H	N	O	S	0	0	0
			3132	1585	593	448	493	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ARG	GLY	CONFLICT	UNP P03437
C	135	ARG	GLY	CONFLICT	UNP P03437
E	135	ARG	GLY	CONFLICT	UNP P03437

- Molecule 2 is a protein called HEMAGGLUTININ, CHAIN HA1.

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		

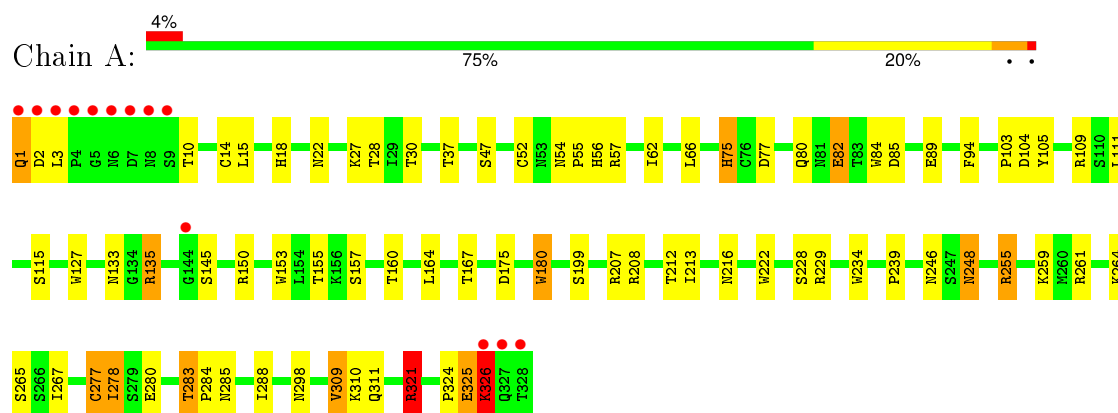
- Molecule 5 is water.

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

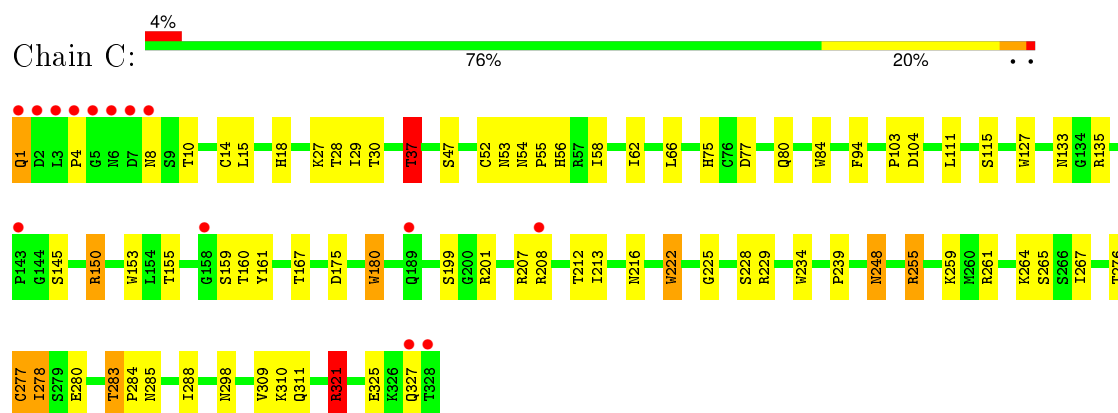
### 3 Residue-property plots

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.

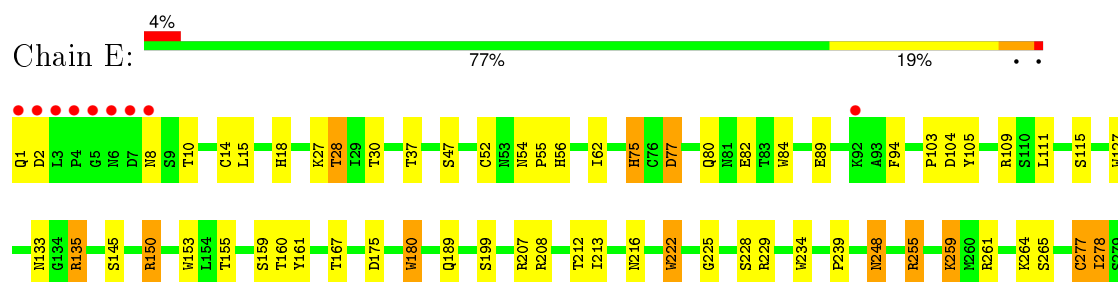
#### • Molecule 1: HEMAGGLUTININ, CHAIN HA1



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

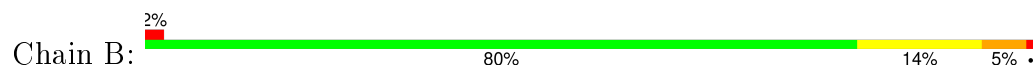


#### • Molecule 1: HEMAGGLUTININ, CHAIN HA1

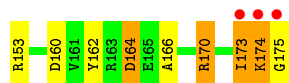
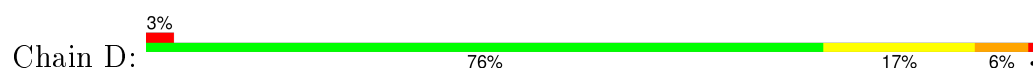




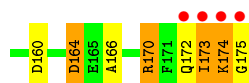
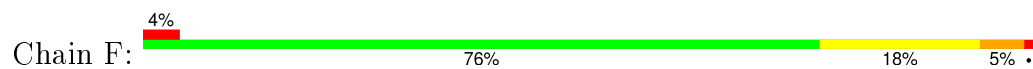
• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1



• Molecule 2: HEMAGGLUTININ, CHAIN HA1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.30Å 163.30Å 176.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.70 17.71 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.70) 62.9 (17.71-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.70Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.224 , (Not available) 0.217 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.0	EDS
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 80085 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2/2596 (0.1%)	1.48	35/3536 (1.0%)
1	C	0.90	1/2596 (0.0%)	1.47	33/3536 (0.9%)
1	E	0.93	2/2596 (0.1%)	1.48	39/3536 (1.1%)
2	B	0.93	0/1445	1.49	20/1939 (1.0%)
2	D	0.95	0/1445	1.50	21/1939 (1.1%)
2	F	0.94	0/1445	1.48	19/1939 (1.0%)
All	All	0.92	5/12123 (0.0%)	1.48	167/16425 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	135	ARG	NE-CZ	7.11	1.42	1.33
1	C	310	LYS	CD-CE	5.69	1.65	1.51
1	A	310	LYS	CD-CE	5.45	1.64	1.51
1	A	234	TRP	CG-CD2	-5.09	1.35	1.43
1	E	310	LYS	CD-CE	5.00	1.63	1.51

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	ARG	NE-CZ-NH2	-13.01	113.79	120.30
1	A	321	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	C	321	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	C	321	ARG	NE-CZ-NH1	12.33	126.47	120.30
1	A	321	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	E	321	ARG	NE-CZ-NH1	11.89	126.24	120.30
2	F	124	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	E	207	ARG	NE-CZ-NH2	-9.52	115.54	120.30
2	B	124	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	E	180	TRP	CD1-CG-CD2	9.32	113.76	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	A	180	TRP	CD1-CG-CD2	8.74	113.29	106.30
1	C	127	TRP	CD1-CG-CD2	8.59	113.17	106.30
2	D	170	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	C	180	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	C	207	ARG	NE-CZ-NH2	-8.49	116.06	120.30
2	B	14	TRP	CD1-CG-CD2	8.44	113.05	106.30
2	D	124	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	E	127	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	C	255	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	B	92	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	C	153	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	127	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	C	222	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	E	222	TRP	CD1-CG-CD2	8.05	112.74	106.30
2	D	92	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	180	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	E	180	TRP	CE2-CD2-CG	-7.90	100.98	107.30
2	B	57	GLU	CA-CB-CG	7.80	130.57	113.40
1	E	153	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	222	TRP	CD1-CG-CD2	7.72	112.48	106.30
2	D	57	GLU	CA-CB-CG	7.70	130.35	113.40
1	E	326	LYS	CA-CB-CG	7.64	130.21	113.40
1	C	127	TRP	CE2-CD2-CG	-7.64	101.19	107.30
2	F	14	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	C	180	TRP	CE2-CD2-CG	-7.61	101.21	107.30
2	F	57	GLU	CA-CB-CG	7.56	130.03	113.40
1	E	255	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	255	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	161	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	E	127	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	E	255	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	153	TRP	CD1-CG-CD2	7.41	112.23	106.30
2	B	170	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	E	84	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	C	234	TRP	CD1-CG-CD2	7.36	112.19	106.30
1	A	127	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	C	255	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	B	92	TRP	CE2-CD2-CG	-7.30	101.46	107.30
2	B	14	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	D	14	TRP	CD1-CG-CD2	7.24	112.09	106.30
2	F	170	ARG	NE-CZ-NH2	-7.24	116.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	TRP	CD1-CG-CD2	7.23	112.08	106.30
2	F	92	TRP	CD1-CG-CD2	7.22	112.08	106.30
2	D	92	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	C	153	TRP	CE2-CD2-CG	-7.19	101.55	107.30
2	F	21	TRP	CD1-CG-CD2	7.18	112.04	106.30
1	C	229	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	E	222	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	A	1	GLN	N-CA-C	-7.07	91.92	111.00
2	D	14	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	E	104	ASP	CB-CG-OD1	7.00	124.60	118.30
1	E	153	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	E	84	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	A	325	GLU	CA-CB-CG	6.91	128.60	113.40
1	A	153	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	C	222	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	E	150	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	150	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	84	TRP	CD1-CG-CD2	6.79	111.73	106.30
2	F	14	TRP	CE2-CD2-CG	-6.71	101.93	107.30
2	D	21	TRP	CD1-CG-CD2	6.65	111.62	106.30
2	B	54	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	C	84	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	A	84	TRP	CE2-CD2-CG	-6.59	102.03	107.30
2	F	92	TRP	CE2-CD2-CG	-6.51	102.10	107.30
1	E	234	TRP	CD1-CG-CD2	6.50	111.50	106.30
1	A	234	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	E	161	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	C	248	ASN	N-CA-CB	-6.49	98.93	110.60
1	A	229	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	E	234	TRP	CE2-CD2-CG	-6.48	102.12	107.30
1	E	180	TRP	CG-CD2-CE3	6.44	139.70	133.90
1	A	222	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	E	180	TRP	CG-CD1-NE1	-6.39	103.70	110.10
2	F	21	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	C	104	ASP	CB-CG-OD1	6.34	124.01	118.30
2	D	54	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	234	TRP	CE2-CD2-CG	-6.32	102.24	107.30
2	D	164	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	255	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	E	229	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	B	164	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	248	ASN	N-CA-CB	-6.17	99.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	TRP	CE2-CD2-CG	-6.14	102.39	107.30
2	D	153	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	21	TRP	CD1-CG-CD2	6.05	111.14	106.30
1	E	1	GLN	N-CA-C	-6.05	94.67	111.00
1	C	1	GLN	N-CA-C	-6.03	94.73	111.00
1	A	180	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	C	180	TRP	CG-CD1-NE1	-5.96	104.14	110.10
1	E	248	ASN	N-CA-CB	-5.95	99.88	110.60
2	D	170	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	B	21	TRP	CE2-CD2-CG	-5.91	102.57	107.30
2	F	25	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	180	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	A	111	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	180	TRP	CG-CD2-CE3	5.79	139.12	133.90
1	E	111	LEU	CA-CB-CG	5.76	128.56	115.30
1	E	150	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	F	54	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	F	124	ARG	CG-CD-NE	-5.73	99.77	111.80
2	D	124	ARG	CG-CD-NE	-5.70	99.83	111.80
2	D	11	GLU	CA-CB-CG	-5.68	100.91	113.40
1	A	104	ASP	CB-CG-OD1	5.66	123.40	118.30
1	E	135	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	180	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	A	208	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	111	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	135	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	E	180	TRP	CB-CG-CD1	-5.54	119.79	127.00
1	A	180	TRP	CB-CG-CD1	-5.51	119.84	127.00
1	C	127	TRP	CG-CD1-NE1	-5.51	104.59	110.10
2	F	164	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	85	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	153	TRP	CG-CD1-NE1	-5.45	104.65	110.10
2	D	141	TYR	CB-CG-CD2	-5.45	117.73	121.00
2	B	14	TRP	CG-CD1-NE1	-5.44	104.66	110.10
2	F	170	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	75	HIS	CA-CB-CG	5.39	122.76	113.60
1	A	127	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	C	150	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	D	21	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	E	208	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	25	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	124	ARG	CG-CD-NE	-5.32	100.63	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	B	127	ARG	CG-CD-NE	-5.28	100.70	111.80
2	D	132	GLU	CA-CB-CG	-5.28	101.79	113.40
2	F	110	LEU	CA-CB-CG	5.27	127.43	115.30
2	B	14	TRP	CG-CD2-CE3	5.26	138.64	133.90
2	F	127	ARG	CG-CD-NE	-5.26	100.75	111.80
1	A	75	HIS	CA-CB-CG	5.24	122.51	113.60
2	F	21	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	E	127	TRP	CG-CD1-NE1	-5.22	104.88	110.10
2	F	132	GLU	CA-CB-CG	-5.22	101.91	113.40
1	A	326	LYS	CA-CB-CG	5.22	124.88	113.40
1	E	105	TYR	CB-CG-CD2	-5.21	117.87	121.00
2	B	132	GLU	CA-CB-CG	-5.20	101.95	113.40
1	E	153	TRP	CG-CD1-NE1	-5.18	104.92	110.10
2	D	110	LEU	CA-CB-CG	5.18	127.20	115.30
1	E	111	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	A	324	PRO	O-C-N	5.15	130.94	122.70
1	E	127	TRP	CG-CD2-CE3	5.15	138.53	133.90
2	D	21	TRP	CE2-CD2-CG	-5.13	103.20	107.30
1	E	28	THR	CA-CB-CG2	5.13	119.58	112.40
1	A	22	ASN	CA-C-N	5.12	126.43	116.20
2	F	51	LYS	N-CA-CB	-5.11	101.40	110.60
1	C	229	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	110	LEU	CA-CB-CG	5.09	127.01	115.30
1	C	208	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	105	TYR	CB-CG-CD2	-5.09	117.95	121.00
2	B	170	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	37	THR	CA-CB-CG2	5.08	119.52	112.40
2	D	162	TYR	CB-CG-CD1	-5.07	117.96	121.00
2	D	127	ARG	CG-CD-NE	-5.05	101.19	111.80
1	E	77	ASP	CB-CG-OD1	5.02	122.81	118.30

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	2539	593	2483	31	0
1	C	2539	593	2483	35	0
1	E	2539	593	2483	32	0
2	B	1421	331	1345	19	0
2	D	1421	331	1345	23	0
2	F	1421	331	1345	23	0
3	A	42	42	39	0	0
3	B	14	14	13	0	0
3	C	42	42	39	0	0
3	D	14	14	13	0	0
3	E	42	42	39	0	0
3	F	14	14	13	0	0
4	A	39	37	34	1	0
4	C	39	37	34	1	0
4	E	39	37	34	1	0
5	A	12	24	0	0	0
5	B	12	24	0	1	0
5	C	11	22	0	1	0
5	D	13	26	0	1	0
5	E	12	24	0	0	0
5	F	12	24	0	1	0
All	All	12237	3195	11742	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.47	0.79
2:D:28:ASN:HB2	2:D:144:CYS:O	1.83	0.78
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.50	0.77
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.48	0.76
2:D:83:TYR:O	2:D:87:THR:HG23	1.87	0.75
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.70	0.74
2:B:83:TYR:O	2:B:87:THR:HG23	1.88	0.73
2:F:83:TYR:O	2:F:87:THR:HG23	1.87	0.73
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.72	0.71
2:B:58:LYS:HE2	2:B:59:THR:O	1.91	0.69
2:D:58:LYS:HE2	2:D:59:THR:O	1.93	0.68
2:F:58:LYS:HE2	2:F:59:THR:O	1.92	0.68
2:B:132:GLU:HG2	2:B:134:GLY:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:GLU:HG2	2:D:134:GLY:H	1.59	0.67
2:F:132:GLU:HG2	2:F:134:GLY:H	1.58	0.67
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.76	0.66
5:B:413:HOH:O	2:F:87:THR:HG22	1.98	0.64
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.82	0.61
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.82	0.61
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.82	0.60
2:B:87:THR:HG22	5:D:402:HOH:O	2.02	0.60
2:D:87:THR:HG22	5:F:403:HOH:O	2.00	0.59
1:A:52:CYS:HB3	1:A:277:CYS:O	2.02	0.59
1:E:52:CYS:HB3	1:E:277:CYS:O	2.02	0.59
1:C:52:CYS:HB3	1:C:277:CYS:O	2.03	0.58
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.86	0.58
2:B:141:TYR:O	2:B:166:ALA:HA	2.05	0.57
2:D:141:TYR:O	2:D:166:ALA:HA	2.04	0.56
1:C:53:ASN:OD1	1:C:276:THR:HA	2.05	0.56
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.87	0.56
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.88	0.56
1:E:283:THR:HG22	1:E:285:ASN:H	1.71	0.56
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.06	0.55
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.06	0.55
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.89	0.55
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.89	0.55
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.87	0.55
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.89	0.55
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.89	0.54
2:F:141:TYR:O	2:F:166:ALA:HA	2.08	0.54
1:A:283:THR:HG22	1:A:285:ASN:H	1.72	0.53
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.08	0.53
1:C:283:THR:HG22	1:C:285:ASN:H	1.73	0.53
1:A:325:GLU:HB2	2:B:13:GLY:O	2.09	0.52
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.25	0.52
1:C:15:LEU:HD22	2:D:119:PHE:HA	1.92	0.51
1:A:10:THR:HG22	2:B:141:TYR:HA	1.93	0.51
1:C:77:ASP:O	1:C:80:GLN:HG3	2.11	0.50
1:E:77:ASP:O	1:E:80:GLN:HG3	2.11	0.50
1:E:47:SER:HA	1:E:288:ILE:HG22	1.93	0.50
1:A:167:THR:HB	4:A:339:NAG:H62	1.94	0.50
1:E:10:THR:HG22	2:F:141:TYR:HA	1.92	0.49
1:E:326:LYS:HD2	1:E:327:GLN:H	1.77	0.49
1:A:75:HIS:HE1	1:A:94:PHE:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.28	0.49
1:E:167:THR:HB	4:E:339:NAG:H62	1.95	0.49
1:C:28:THR:HG22	1:C:30:THR:H	1.78	0.49
1:C:75:HIS:HE1	1:C:94:PHE:O	1.95	0.48
1:A:47:SER:HA	1:A:288:ILE:HG22	1.94	0.48
1:C:10:THR:HG22	2:D:141:TYR:HA	1.94	0.48
1:E:28:THR:HG22	1:E:30:THR:H	1.79	0.48
1:C:47:SER:HA	1:C:288:ILE:HG22	1.94	0.48
1:A:28:THR:HG22	1:A:30:THR:H	1.78	0.48
1:E:75:HIS:HE1	1:E:94:PHE:O	1.97	0.48
1:C:135:ARG:HG3	1:C:145:SER:HB2	1.96	0.48
1:A:77:ASP:O	1:A:80:GLN:HG3	2.13	0.48
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.62	0.47
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.63	0.47
1:C:167:THR:HB	4:C:339:NAG:H62	1.95	0.47
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.97	0.47
1:A:135:ARG:HG3	1:A:145:SER:HB2	1.97	0.46
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.63	0.46
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.31	0.46
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.47	0.45
2:F:127:ARG:HB3	2:F:128:GLU:H	1.67	0.45
2:B:54:ARG:NH2	1:E:27:LYS:HD3	2.30	0.45
2:D:87:THR:HG21	2:F:88:LYS:HD2	1.98	0.45
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.81	0.45
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.82	0.45
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.82	0.44
2:B:127:ARG:HB3	2:B:128:GLU:H	1.66	0.44
1:E:54:ASN:O	1:E:278:ILE:HA	2.18	0.44
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.17	0.44
2:D:91:LEU:HD13	2:F:91:LEU:HD13	2.00	0.44
1:C:27:LYS:HD3	2:F:54:ARG:NH2	2.33	0.44
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.18	0.43
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.17	0.43
1:A:66:LEU:HD22	1:A:267:ILE:HD12	2.01	0.43
2:D:135:ASN:OD1	2:D:135:ASN:N	2.52	0.43
1:C:135:ARG:NH1	1:C:145:SER:O	2.52	0.43
1:C:325:GLU:HG2	1:C:325:GLU:O	2.19	0.43
2:F:20:GLY:HA3	2:F:36:ALA:HB1	2.00	0.43
1:C:14:CYS:HA	2:D:137:CYS:HA	2.01	0.43
2:B:114:GLU:OE2	2:B:117:LYS:NZ	2.52	0.43
1:A:54:ASN:O	1:A:278:ILE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD22	1:C:267:ILE:HD12	2.01	0.42
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.19	0.42
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.69	0.42
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.52	0.42
2:D:26:HIS:ND1	2:D:149:ILE:HG21	2.35	0.42
1:C:115:SER:O	1:C:261:ARG:HG3	2.19	0.42
1:E:28:THR:HG23	2:F:105:GLN:OE1	2.19	0.42
1:A:27:LYS:HD3	2:D:54:ARG:NH2	2.34	0.42
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.53	0.42
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.52	0.42
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.20	0.41
1:A:14:CYS:HA	2:B:137:CYS:HA	2.02	0.41
1:C:54:ASN:O	1:C:278:ILE:HA	2.20	0.41
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.35	0.41
1:C:15:LEU:HD23	2:D:118:LEU:HG	2.03	0.41
2:D:20:GLY:HA3	2:D:36:ALA:HB1	2.02	0.41
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.52	0.41
1:E:115:SER:O	1:E:261:ARG:HG3	2.20	0.41
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.41
1:C:37:THR:HG21	5:C:352:HOH:O	2.21	0.41
1:A:164:LEU:O	1:A:246:ASN:HA	2.20	0.41
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.52	0.41
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.54	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.02	0.41
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.36	0.41
2:D:127:ARG:HB3	2:D:128:GLU:H	1.65	0.41
1:E:326:LYS:HD2	1:E:327:GLN:N	2.36	0.41
1:C:284:PRO:HG2	1:C:298:ASN:ND2	2.36	0.41
1:E:135:ARG:HG3	1:E:145:SER:HB2	2.02	0.41
1:C:29:ILE:HB	2:D:105:GLN:OE1	2.21	0.41
1:C:201:ARG:HH11	1:C:201:ARG:HD3	1.79	0.40
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.56	0.40
2:F:26:HIS:O	2:F:32:THR:HA	2.20	0.40
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.54	0.40
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.56	0.40
1:A:115:SER:O	1:A:261:ARG:HG3	2.22	0.40
2:B:20:GLY:HA3	2:B:36:ALA:HB1	2.03	0.40
1:A:284:PRO:HG2	1:A:298:ASN:ND2	2.36	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%)	303 (93%)	19 (6%)	4 (1%)	16	39
1	C	326/328 (99%)	306 (94%)	17 (5%)	3 (1%)	21	49
1	E	326/328 (99%)	309 (95%)	16 (5%)	1 (0%)	46	75
2	B	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	11	29
2	D	173/175 (99%)	162 (94%)	8 (5%)	3 (2%)	11	29
2	F	173/175 (99%)	161 (93%)	8 (5%)	4 (2%)	8	20
All	All	1497/1509 (99%)	1402 (94%)	77 (5%)	18 (1%)	16	39

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
1	C	327	GLN
2	D	58	LYS
2	D	173	ILE
2	F	58	LYS
2	F	173	ILE
1	A	2	ASP
1	A	62	ILE
1	C	62	ILE
2	D	174	LYS
1	E	62	ILE
2	F	174	LYS
2	B	174	LYS
1	C	4	PRO
2	F	172	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	290/290 (100%)	269 (93%)	21 (7%)	18	41
1	C	290/290 (100%)	271 (93%)	19 (7%)	21	45
1	E	290/290 (100%)	268 (92%)	22 (8%)	16	37
2	B	149/149 (100%)	143 (96%)	6 (4%)	38	69
2	D	149/149 (100%)	142 (95%)	7 (5%)	32	63
2	F	149/149 (100%)	142 (95%)	7 (5%)	32	63
All	All	1317/1317 (100%)	1235 (94%)	82 (6%)	23	49

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	18	HIS
1	A	37	THR
1	A	82	GLU
1	A	103	PRO
1	A	150	ARG
1	A	155	THR
1	A	157	SER
1	A	160	THR
1	A	199	SER
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	309	VAL
1	A	321	ARG
1	A	326	LYS
2	B	87	THR

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Mol	Chain	Res	Type
2	B	110	LEU
2	B	127	ARG
2	B	145	ASP
2	B	160	ASP
2	B	170	ARG
1	C	8	ASN
1	C	18	HIS
1	C	37	THR
1	C	58	ILE
1	C	103	PRO
1	C	150	ARG
1	C	155	THR
1	C	159	SER
1	C	160	THR
1	C	199	SER
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	321	ARG
2	D	87	THR
2	D	110	LEU
2	D	127	ARG
2	D	145	ASP
2	D	150	GLU
2	D	160	ASP
2	D	170	ARG
1	E	2	ASP
1	E	8	ASN
1	E	18	HIS
1	E	37	THR
1	E	82	GLU
1	E	103	PRO
1	E	150	ARG
1	E	155	THR
1	E	159	SER
1	E	160	THR
1	E	189	GLN

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Mol	Chain	Res	Type
1	E	199	SER
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	321	ARG
1	E	326	LYS
2	F	11	GLU
2	F	110	LEU
2	F	127	ARG
2	F	128	GLU
2	F	145	ASP
2	F	160	ASP
2	F	170	ARG

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

Mol	Chain	Res	Type
1	A	132	GLN
1	A	171	ASN
1	C	132	GLN
1	C	171	ASN
1	E	132	GLN
1	E	171	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

9 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	14,14,15	0.62	0	15,19,21	0.79	0
4	NAG	A	340	4	14,14,15	0.60	0	15,19,21	1.19	1 (6%)
4	BMA	A	341	4	11,11,12	0.55	0	14,15,17	1.28	1 (7%)
4	NAG	C	339	1,4	14,14,15	0.91	1 (7%)	15,19,21	0.88	0
4	NAG	C	340	4	14,14,15	0.50	0	15,19,21	1.16	1 (6%)
4	BMA	C	341	4	11,11,12	0.49	0	14,15,17	1.43	3 (21%)
4	NAG	E	339	1,4	14,14,15	0.63	0	15,19,21	0.88	0
4	NAG	E	340	4	14,14,15	0.44	0	15,19,21	1.07	1 (6%)
4	BMA	E	341	4	11,11,12	0.77	0	14,15,17	0.89	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	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
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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	339	NAG	O5-C1	-2.17	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	340	NAG	C4-C3-C2	-2.91	106.70	111.23
4	C	340	NAG	C4-C3-C2	-2.64	107.12	111.23
4	E	340	NAG	C4-C3-C2	-2.59	107.20	111.23
4	C	341	BMA	C6-C5-C4	-2.54	106.74	113.02
4	C	341	BMA	O5-C1-C2	-2.54	106.74	110.86
4	A	341	BMA	C1-O5-C5	2.78	115.77	112.25
4	C	341	BMA	C1-O5-C5	3.06	116.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	339	NAG	1	0
4	C	339	NAG	1	0
4	E	339	NAG	1	0

## 5.6 Ligand geometry [i](#)

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	14,14,15	0.77	1 (7%)	15,19,21	1.04	0
3	NAG	A	334	1	14,14,15	0.80	0	15,19,21	1.09	1 (6%)
3	NAG	A	348	1	14,14,15	0.58	0	15,19,21	1.66	4 (26%)
3	NAG	B	401	2	14,14,15	0.66	0	15,19,21	1.43	1 (6%)
3	NAG	C	329	1	14,14,15	0.70	1 (7%)	15,19,21	1.10	2 (13%)
3	NAG	C	334	1	14,14,15	0.73	0	15,19,21	1.04	1 (6%)
3	NAG	C	348	1	14,14,15	0.67	0	15,19,21	1.66	4 (26%)
3	NAG	D	401	2	14,14,15	0.70	0	15,19,21	1.47	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	329	1	14,14,15	0.70	0	15,19,21	1.11	1 (6%)
3	NAG	E	334	1	14,14,15	0.75	0	15,19,21	0.97	1 (6%)
3	NAG	E	348	1	14,14,15	0.61	0	15,19,21	1.65	3 (20%)
3	NAG	F	401	2	14,14,15	0.72	0	15,19,21	1.49	1 (6%)

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	C	329	NAG	C4-C5	2.19	1.57	1.53
3	A	329	NAG	C4-C5	2.28	1.57	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	348	NAG	C3-C4-C5	-2.43	105.96	110.20
3	E	348	NAG	C3-C4-C5	-2.40	106.01	110.20
3	A	348	NAG	C3-C4-C5	-2.13	106.48	110.20
3	C	329	NAG	O4-C4-C3	-2.07	105.69	110.34
3	C	348	NAG	O4-C4-C5	2.07	114.72	109.24
3	C	329	NAG	C1-O5-C5	2.10	114.91	112.25
3	A	348	NAG	O4-C4-C5	2.16	114.96	109.24
3	C	334	NAG	C1-O5-C5	2.42	115.32	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	348	NAG	C8-C7-N2	2.43	120.75	116.11
3	E	348	NAG	C8-C7-N2	2.49	120.87	116.11
3	E	334	NAG	C1-O5-C5	2.49	115.41	112.25
3	E	329	NAG	C1-O5-C5	2.54	115.47	112.25
3	C	348	NAG	C8-C7-N2	2.71	121.28	116.11
3	A	334	NAG	C1-O5-C5	2.98	116.03	112.25
3	C	348	NAG	C1-O5-C5	3.76	117.02	112.25
3	E	348	NAG	C1-O5-C5	4.03	117.36	112.25
3	A	348	NAG	C1-O5-C5	4.20	117.57	112.25
3	B	401	NAG	C1-O5-C5	4.22	117.60	112.25
3	D	401	NAG	C1-O5-C5	4.48	117.94	112.25
3	F	401	NAG	C1-O5-C5	4.61	118.10	112.25

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 [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

### 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%)	-0.15	13 (3%)	42	41	10, 28, 54, 149	0
1	C	328/328 (100%)	-0.11	14 (4%)	39	38	10, 28, 53, 154	0
1	E	328/328 (100%)	-0.11	12 (3%)	45	45	9, 27, 54, 149	0
2	B	175/175 (100%)	-0.39	4 (2%)	64	64	3, 22, 56, 107	0
2	D	175/175 (100%)	-0.38	6 (3%)	49	49	3, 22, 54, 107	0
2	F	175/175 (100%)	-0.42	7 (4%)	42	41	3, 22, 54, 107	0
All	All	1509/1509 (100%)	-0.22	56 (3%)	45	45	3, 26, 55, 154	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	14.0
1	C	7	ASP	10.6
1	E	4	PRO	10.5
1	A	328	THR	10.4
1	C	5	GLY	9.9
2	D	175	GLY	9.6
1	A	3	LEU	9.5
1	C	3	LEU	9.3
1	E	7	ASP	9.2
1	E	6	ASN	9.0
1	C	8	ASN	8.9
1	C	4	PRO	8.9
1	E	2	ASP	8.6
1	A	8	ASN	8.6
1	A	6	ASN	8.5
1	E	3	LEU	8.5
1	E	1	GLN	8.3
1	C	6	ASN	8.3
1	A	5	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
2	B	175	GLY	7.8
2	F	175	GLY	7.7
1	A	327	GLN	7.7
1	C	2	ASP	7.6
1	E	328	THR	7.4
1	E	327	GLN	7.2
2	B	174	LYS	6.9
1	A	2	ASP	6.7
2	D	173	ILE	6.6
1	C	328	THR	6.4
1	E	5	GLY	6.3
1	A	4	PRO	6.3
1	C	1	GLN	5.8
2	F	173	ILE	5.7
2	F	174	LYS	5.2
1	A	1	GLN	4.9
2	B	173	ILE	4.8
1	A	326	LYS	4.8
2	D	174	LYS	4.4
2	D	58	LYS	4.0
1	E	8	ASN	3.8
2	F	58	LYS	3.0
1	C	327	GLN	2.8
1	C	208	ARG	2.8
1	C	158	GLY	2.7
1	E	326	LYS	2.6
1	C	143	PRO	2.6
2	D	57	GLU	2.5
2	B	58	LYS	2.5
2	F	57	GLU	2.3
2	F	172	GLN	2.3
1	C	189	GLN	2.3
1	A	144	GLY	2.3
1	E	92	LYS	2.3
2	D	143	LYS	2.2
1	A	9	SER	2.2
2	F	59	THR	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	340	14/15	0.92	0.18	0.15	0,0,56,60	0
4	NAG	A	340	14/15	0.93	0.17	-0.04	0,0,57,59	0
4	NAG	A	339	14/15	0.94	0.15	-0.08	0,0,45,49	0
4	NAG	E	340	14/15	0.90	0.19	-0.23	0,0,57,60	0
4	NAG	C	339	14/15	0.91	0.15	-0.44	0,0,45,48	0
4	NAG	E	339	14/15	0.96	0.12	-0.91	0,0,44,48	0
4	BMA	C	341	11/12	0.87	0.38	-	0,0,67,69	0
4	BMA	A	341	11/12	0.80	0.28	-	0,0,64,67	0
4	BMA	E	341	11/12	0.81	0.31	-	0,0,67,69	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	329	14/15	0.91	0.27	7.91	0,0,51,51	0
3	NAG	D	401	14/15	0.82	0.38	7.86	0,0,67,67	0
3	NAG	E	348	14/15	0.92	0.30	7.77	0,0,50,51	0
3	NAG	E	329	14/15	0.90	0.30	6.93	0,0,51,52	0
3	NAG	A	329	14/15	0.90	0.25	6.85	0,0,51,52	0
3	NAG	B	401	14/15	0.85	0.34	5.66	0,0,67,67	0
3	NAG	C	348	14/15	0.87	0.30	5.06	0,0,50,51	0
3	NAG	F	401	14/15	0.89	0.28	3.99	0,0,67,67	0
3	NAG	A	348	14/15	0.92	0.22	3.60	0,0,49,52	0
3	NAG	C	334	14/15	0.84	0.28	3.35	0,0,49,51	0
3	NAG	E	334	14/15	0.93	0.21	2.24	0,0,48,51	0
3	NAG	A	334	14/15	0.93	0.21	1.60	0,0,48,50	0

## 6.5 Other polymers

There are no such residues in this entry.