



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:01 AM GMT

PDB ID : 1HGE  
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 : 2.60 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>

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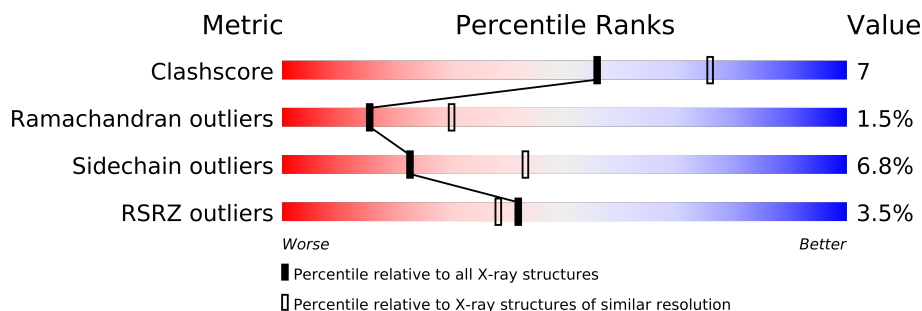
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	348	-	X
3	NAG	B	401	-	X
3	NAG	C	329	-	X
3	NAG	C	334	-	X

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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
3	NAG	F	401	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15549 atoms, of which 3246 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, (G135R), HA1 CHAIN.

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, (G135R), HA1 CHAIN.

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		

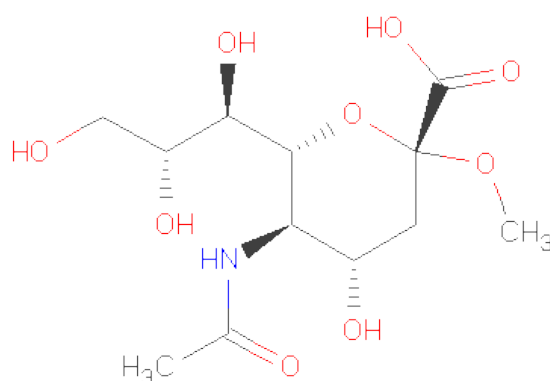
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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		

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 5 is 2-O-METHYL-5-N-ACETYL-ALPHA-D-NEURAMINIC ACID (three-letter code: MNA) (formula:  $C_{12}H_{21}NO_9$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	C	1	Total	C	H	N	O	0	0
			39	12	17	1	9		
5	E	1	Total	C	H	N	O	0	0
			39	12	17	1	9		

- Molecule 6 is water.

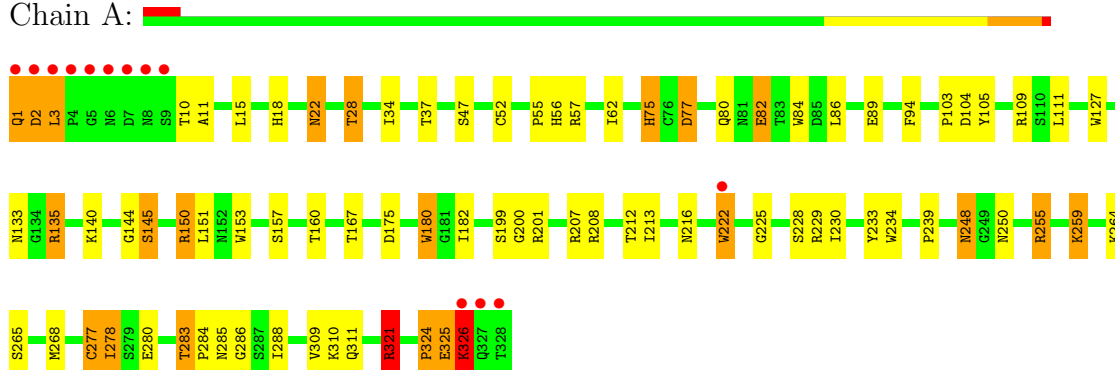
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	11	Total 33	H 22	O 11	0	0
6	B	13	Total 39	H 26	O 13	0	0
6	C	11	Total 33	H 22	O 11	0	0
6	D	13	Total 39	H 26	O 13	0	0
6	E	11	Total 33	H 22	O 11	0	0
6	F	13	Total 39	H 26	O 13	0	0

### 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.

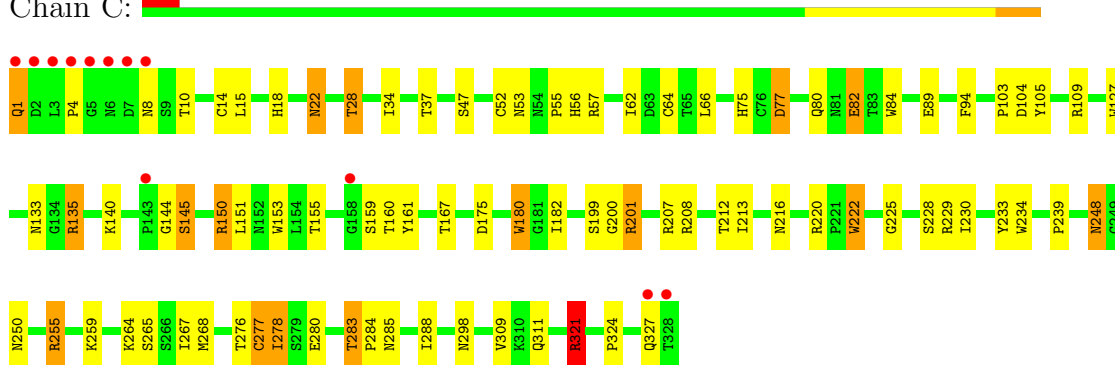
- Molecule 1: HEMAGGLUTININ, (G135R), HA1 CHAIN

Chain A:



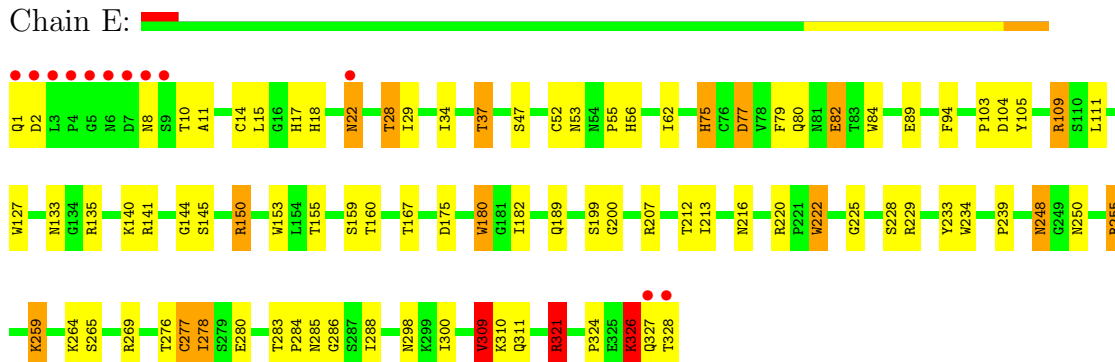
- Molecule 1: HEMAGGLUTININ, (G135R), HA1 CHAIN

Chain C:



- Molecule 1: HEMAGGLUTININ, (G135R), HA1 CHAIN

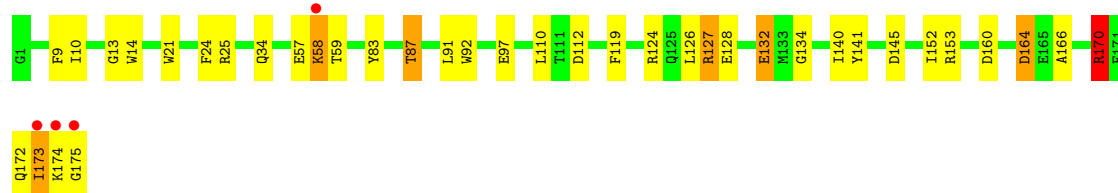
Chain E:





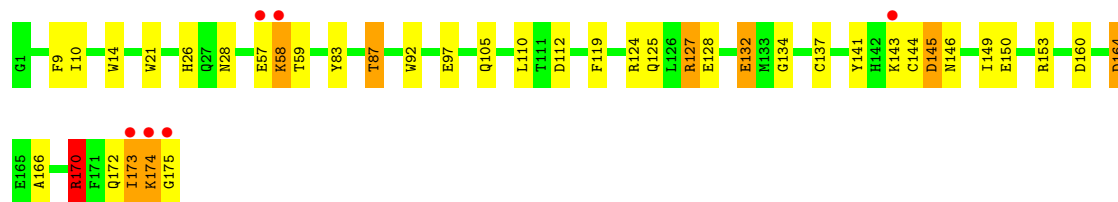
- Molecule 2: HEMAGGLUTININ, (G135R), HA1 CHAIN

Chain B: 



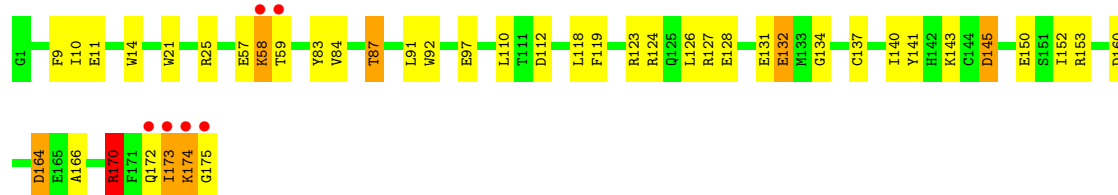
- Molecule 2: HEMAGGLUTININ, (G135R), HA1 CHAIN

Chain D: 



- Molecule 2: HEMAGGLUTININ, (G135R), HA1 CHAIN

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.10Å 163.10Å 176.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60 15.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.60) 54.1 (15.92-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.62Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.225 , (Not available) 0.226 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 18.0	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 76215 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15549	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 2.72% 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: MNA, 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	3/2596 (0.1%)	1.49	41/3536 (1.2%)
1	C	0.90	1/2596 (0.0%)	1.50	41/3536 (1.2%)
1	E	0.93	2/2596 (0.1%)	1.50	41/3536 (1.2%)
2	B	0.93	0/1445	1.44	14/1939 (0.7%)
2	D	0.95	0/1445	1.47	19/1939 (1.0%)
2	F	0.93	0/1445	1.46	19/1939 (1.0%)
All	All	0.92	6/12123 (0.0%)	1.48	175/16425 (1.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	135	ARG	NE-CZ	7.82	1.43	1.33
1	A	135	ARG	NE-CZ	5.30	1.40	1.33
1	A	234	TRP	CG-CD2	-5.28	1.34	1.43
1	C	135	ARG	NE-CZ	5.23	1.39	1.33
1	E	310	LYS	CD-CE	5.08	1.64	1.51
1	A	310	LYS	CD-CE	5.02	1.63	1.51

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	ARG	NE-CZ-NH2	-14.42	113.09	120.30
1	E	321	ARG	NE-CZ-NH2	-13.77	113.41	120.30
1	A	321	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	C	321	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	A	321	ARG	NE-CZ-NH1	11.63	126.12	120.30
1	E	321	ARG	NE-CZ-NH1	11.15	125.88	120.30
2	F	124	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	E	135	ARG	NE-CZ-NH2	-10.68	114.96	120.30
2	B	124	ARG	NE-CZ-NH2	-9.61	115.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	124	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	E	207	ARG	NE-CZ-NH2	-9.14	115.73	120.30
2	D	92	TRP	CD1-CG-CD2	9.08	113.57	106.30
1	E	180	TRP	CD1-CG-CD2	8.89	113.41	106.30
1	A	180	TRP	CD1-CG-CD2	8.84	113.37	106.30
2	B	92	TRP	CD1-CG-CD2	8.83	113.37	106.30
1	A	207	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	E	222	TRP	CD1-CG-CD2	8.59	113.17	106.30
1	C	180	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	E	255	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	222	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	C	229	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	F	21	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	C	207	ARG	NE-CZ-NH2	-8.24	116.18	120.30
2	B	14	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	C	127	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	222	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	D	170	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	F	14	TRP	CD1-CG-CD2	7.91	112.63	106.30
1	A	180	TRP	CE2-CD2-CG	-7.88	101.00	107.30
2	F	92	TRP	CD1-CG-CD2	7.88	112.60	106.30
2	B	170	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	E	180	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	127	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	E	255	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	D	14	TRP	CD1-CG-CD2	7.54	112.33	106.30
2	B	92	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	C	153	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	C	127	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	A	229	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	E	222	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	E	326	LYS	CA-CB-CG	7.36	129.58	113.40
1	C	255	ARG	NE-CZ-NH1	7.33	123.96	120.30
2	B	57	GLU	CA-CB-CG	7.30	129.46	113.40
1	C	180	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	234	TRP	CD1-CG-CD2	7.27	112.12	106.30
2	F	57	GLU	CA-CB-CG	7.27	129.39	113.40
1	A	325	GLU	CA-CB-CG	7.26	129.38	113.40
2	D	57	GLU	CA-CB-CG	7.24	129.32	113.40
2	B	14	TRP	CE2-CD2-CG	-7.21	101.53	107.30
2	F	170	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	E	229	ARG	NE-CZ-NH2	-7.21	116.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	TYR	CB-CG-CD2	-7.20	116.68	121.00
2	D	92	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	C	150	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	E	234	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	E	127	TRP	CD1-CG-CD2	7.14	112.01	106.30
2	D	21	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	A	1	GLN	N-CA-C	-7.06	91.94	111.00
1	C	135	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	234	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	A	127	TRP	CE2-CD2-CG	-7.02	101.69	107.30
1	C	255	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	D	14	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	E	84	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	E	153	TRP	CD1-CG-CD2	6.94	111.85	106.30
1	C	222	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	E	234	TRP	CD1-CG-CD2	6.93	111.84	106.30
2	F	92	TRP	CE2-CD2-CG	-6.82	101.84	107.30
2	F	21	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	A	153	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	C	153	TRP	CE2-CD2-CG	-6.78	101.88	107.30
2	F	14	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	A	222	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	234	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	C	84	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	E	84	TRP	CE2-CD2-CG	-6.67	101.97	107.30
1	A	255	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	B	21	TRP	CD1-CG-CD2	6.63	111.61	106.30
1	C	84	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	C	234	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	A	84	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	E	180	TRP	CG-CD2-CE3	6.47	139.72	133.90
1	E	229	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	E	127	TRP	CE2-CD2-CG	-6.45	102.14	107.30
1	E	104	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	104	ASP	CB-CG-OD1	6.40	124.06	118.30
2	D	153	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	E	153	TRP	CE2-CD2-CG	-6.36	102.22	107.30
2	B	21	TRP	CE2-CD2-CG	-6.32	102.25	107.30
1	A	84	TRP	CD1-CG-CD2	6.32	111.35	106.30
2	D	112	ASP	CB-CG-OD1	6.26	123.94	118.30
1	E	150	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	153	TRP	CE2-CD2-CG	-6.16	102.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	324	PRO	O-C-N	6.08	132.42	122.70
1	E	1	GLN	N-CA-C	-6.08	94.59	111.00
1	C	1	GLN	N-CA-C	-6.05	94.66	111.00
1	E	269	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	180	TRP	CB-CG-CD1	-6.01	119.19	127.00
1	A	180	TRP	CG-CD2-CE3	6.00	139.31	133.90
1	A	104	ASP	CB-CG-OD1	6.00	123.69	118.30
1	E	180	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	A	255	ARG	NE-CZ-NH1	5.97	123.28	120.30
2	F	132	GLU	CA-CB-CG	-5.96	100.30	113.40
1	C	248	ASN	N-CA-CB	-5.95	99.88	110.60
2	B	132	GLU	CA-CB-CG	-5.94	100.34	113.40
2	F	112	ASP	CB-CG-OD1	5.92	123.62	118.30
2	D	132	GLU	CA-CB-CG	-5.89	100.45	113.40
1	E	28	THR	CA-CB-CG2	5.88	120.64	112.40
1	A	321	ARG	CB-CG-CD	-5.88	96.32	111.60
1	C	180	TRP	CG-CD2-CE3	5.87	139.18	133.90
1	E	321	ARG	CB-CG-CD	-5.87	96.34	111.60
2	F	21	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	C	105	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	C	321	ARG	CB-CG-CD	-5.86	96.37	111.60
1	E	105	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	180	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	C	82	GLU	N-CA-CB	-5.80	100.15	110.60
1	E	220	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	E	135	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	150	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	D	21	TRP	CE2-CD2-CG	-5.71	102.73	107.30
2	B	112	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	248	ASN	N-CA-CB	-5.68	100.38	110.60
2	F	110	LEU	CA-CB-CG	5.68	128.36	115.30
2	B	164	ASP	CB-CG-OD2	5.62	123.36	118.30
2	D	164	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	248	ASN	N-CA-CB	-5.60	100.52	110.60
1	C	82	GLU	CA-CB-CG	5.60	125.72	113.40
1	E	180	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	C	180	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	180	TRP	CB-CG-CD1	-5.48	119.88	127.00
2	B	92	TRP	CG-CD1-NE1	-5.48	104.62	110.10
2	D	92	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	C	77	ASP	CB-CG-OD1	5.44	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	25	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	208	ARG	NE-CZ-NH2	-5.39	117.60	120.30
2	F	84	VAL	CA-CB-CG2	-5.38	102.82	110.90
1	E	75	HIS	CA-CB-CG	5.34	122.69	113.60
2	F	123	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	229	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	208	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	105	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	22	ASN	CA-C-N	5.26	126.72	116.20
1	A	28	THR	CA-CB-CG2	5.23	119.72	112.40
1	C	153	TRP	CG-CD1-NE1	-5.22	104.88	110.10
2	D	21	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	E	77	ASP	CB-CG-OD1	5.19	122.97	118.30
2	D	146	ASN	CB-CA-C	-5.18	100.04	110.40
1	C	127	TRP	CG-CD1-NE1	-5.17	104.93	110.10
2	D	110	LEU	CA-CB-CG	5.16	127.18	115.30
1	E	207	ARG	CG-CD-NE	-5.15	100.98	111.80
1	C	220	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	324	PRO	CA-C-N	-5.14	105.89	117.20
1	C	22	ASN	CA-C-N	5.14	126.48	116.20
1	E	22	ASN	CA-C-N	5.14	126.47	116.20
2	F	124	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	207	ARG	CG-CD-NE	-5.13	101.03	111.80
1	C	64	CYS	CA-CB-SG	-5.11	104.79	114.00
1	E	111	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	111	LEU	CA-CB-CG	5.11	127.06	115.30
1	C	201	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	75	HIS	CA-CB-CG	5.06	122.19	113.60
1	A	201	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	326	LYS	CA-CB-CG	5.04	124.49	113.40
2	F	164	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	109	ARG	NE-CZ-NH1	-5.03	117.78	120.30
2	D	125	GLN	N-CA-CB	-5.02	101.56	110.60
1	A	153	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	C	222	TRP	CG-CD1-NE1	-5.01	105.09	110.10
2	F	25	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	E	309	VAL	N-CA-CB	-5.01	100.47	111.50
2	B	110	LEU	CA-CB-CG	5.01	126.82	115.30
2	D	124	ARG	CG-CD-NE	-5.00	101.29	111.80
1	A	77	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2539	593	1894	38	0
1	C	2539	593	1894	39	0
1	E	2539	593	1894	42	0
2	B	1421	331	1015	22	0
2	D	1421	331	1015	21	0
2	F	1421	331	1015	21	0
3	A	42	42	0	0	0
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	1	0
4	E	39	37	0	1	0
5	A	22	17	3	0	0
5	C	22	17	1	0	0
5	E	22	17	1	0	0
6	A	11	22	0	0	0
6	B	13	26	0	1	0
6	C	11	22	0	0	0
6	D	13	26	0	2	0
6	E	11	22	0	2	0
6	F	13	26	0	2	0
All	All	12303	3246	8732	159	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 (159) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:83:TYR:O	2:B:87:THR:HG23	1.86	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:321:ARG:HG2	1:E:321:ARG:HH11	1.53	0.74
2:F:83:TYR:O	2:F:87:THR:HG23	1.86	0.73
2:D:83:TYR:O	2:D:87:THR:HG23	1.89	0.73
1:C:216:ASN:HB3	1:E:212:THR:HG21	1.70	0.73
2:B:58:LYS:HE2	2:B:59:THR:O	1.88	0.72
1:C:321:ARG:HH11	1:C:321:ARG:HG2	1.55	0.72
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.55	0.70
2:D:58:LYS:HE2	2:D:59:THR:O	1.90	0.70
2:F:58:LYS:HE2	2:F:59:THR:O	1.90	0.70
2:B:164:ASP:HB3	2:F:175:GLY:HA3	1.74	0.70
2:D:28:ASN:HB2	2:D:144:CYS:O	1.96	0.66
2:B:175:GLY:HA3	2:D:164:ASP:HB3	1.76	0.65
2:D:173:ILE:HG22	2:D:174:LYS:HG2	1.80	0.63
2:B:173:ILE:HG22	2:B:174:LYS:HG2	1.80	0.62
2:F:173:ILE:HG22	2:F:174:LYS:HG2	1.81	0.62
6:B:414:HOH:O	2:F:87:THR:HG22	2.01	0.61
1:A:325:GLU:HB2	2:B:13:GLY:O	2.02	0.59
2:D:87:THR:HG22	6:F:403:HOH:O	2.02	0.58
1:E:37:THR:HG21	6:E:352:HOH:H1	1.69	0.57
1:E:79:PHE:O	1:E:82:GLU:HB2	2.05	0.57
2:B:141:TYR:O	2:B:166:ALA:HA	2.05	0.56
1:A:212:THR:HG21	1:E:216:ASN:HB3	1.86	0.56
2:D:175:GLY:HA3	2:F:164:ASP:HB3	1.86	0.56
2:D:141:TYR:O	2:D:166:ALA:HA	2.06	0.55
1:A:55:PRO:HD3	1:A:278:ILE:HD12	1.89	0.55
2:B:132:GLU:HG2	2:B:134:GLY:H	1.72	0.55
1:E:55:PRO:HD3	1:E:278:ILE:HD12	1.89	0.55
2:D:26:HIS:HD1	6:D:408:HOH:H2	1.56	0.54
2:F:132:GLU:HG2	2:F:134:GLY:H	1.72	0.54
1:E:52:CYS:HB3	1:E:277:CYS:O	2.08	0.54
2:D:132:GLU:HG2	2:D:134:GLY:H	1.72	0.53
1:E:311:GLN:NE2	2:F:97:GLU:HB2	2.24	0.53
1:C:52:CYS:HB3	1:C:277:CYS:O	2.09	0.53
2:F:141:TYR:O	2:F:166:ALA:HA	2.08	0.53
1:C:55:PRO:HD3	1:C:278:ILE:HD12	1.90	0.52
1:E:300:ILE:HA	6:F:412:HOH:H2	1.76	0.51
1:E:10:THR:HG22	2:F:141:TYR:HA	1.91	0.51
1:C:180:TRP:HH2	1:C:213:ILE:HD13	1.75	0.51
1:A:216:ASN:HB3	1:C:212:THR:HG21	1.91	0.51
2:B:87:THR:HG22	6:D:402:HOH:O	2.11	0.51
1:A:182:ILE:HD13	1:A:213:ILE:HG22	1.92	0.51
1:E:180:TRP:HH2	1:E:213:ILE:HD13	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:THR:HG22	2:B:141:TYR:HA	1.93	0.50
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.11	0.50
1:A:52:CYS:HB3	1:A:277:CYS:O	2.11	0.49
1:A:56:HIS:ND1	1:A:264:LYS:NZ	2.60	0.49
1:E:56:HIS:ND1	1:E:264:LYS:NZ	2.60	0.49
1:C:10:THR:HG22	2:D:141:TYR:HA	1.94	0.49
1:C:182:ILE:HD13	1:C:213:ILE:HG22	1.94	0.49
1:C:56:HIS:ND1	1:C:264:LYS:NZ	2.60	0.49
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.48	0.49
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.48	0.49
1:C:311:GLN:NE2	2:D:97:GLU:HB2	2.29	0.48
1:E:309:VAL:HG13	1:E:311:GLN:OE1	2.13	0.48
1:A:311:GLN:NE2	2:B:97:GLU:HB2	2.29	0.48
1:A:309:VAL:HG13	1:A:311:GLN:OE1	2.14	0.48
1:E:182:ILE:HD13	1:E:213:ILE:HG22	1.95	0.48
1:C:222:TRP:CE2	1:C:225:GLY:HA2	2.49	0.48
1:A:180:TRP:HH2	1:A:213:ILE:HD13	1.78	0.47
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.14	0.47
1:C:135:ARG:NH1	1:C:145:SER:O	2.48	0.47
1:C:53:ASN:OD1	1:C:276:THR:HA	2.14	0.47
1:A:167:THR:HB	4:A:339:NAG:H62	1.97	0.47
1:E:140:LYS:HG3	1:E:144:GLY:O	2.15	0.46
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.15	0.46
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.48	0.46
1:E:326:LYS:HB3	1:E:326:LYS:HE3	1.67	0.46
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.15	0.46
1:E:77:ASP:O	1:E:80:GLN:HG3	2.16	0.46
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.50	0.46
1:E:75:HIS:HE1	1:E:94:PHE:O	1.99	0.46
1:C:77:ASP:O	1:C:80:GLN:HG3	2.16	0.46
1:C:140:LYS:HG3	1:C:144:GLY:O	2.15	0.46
1:C:167:THR:HB	4:C:339:NAG:H62	1.98	0.46
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.98	0.46
1:A:89:GLU:OE1	1:A:109:ARG:NH1	2.49	0.45
1:E:167:THR:HB	4:E:339:NAG:H62	1.98	0.45
1:A:140:LYS:HG3	1:A:144:GLY:O	2.16	0.45
1:A:75:HIS:HE1	1:A:94:PHE:O	1.98	0.45
1:A:268:MET:SD	1:A:284:PRO:HD3	2.57	0.45
2:B:127:ARG:HB3	2:B:128:GLU:H	1.65	0.45
1:C:283:THR:HG22	1:C:285:ASN:H	1.82	0.45
1:C:75:HIS:HE1	1:C:94:PHE:O	1.99	0.45
1:E:283:THR:HB	1:E:286:GLY:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.99	0.45
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.52	0.45
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.16	0.45
2:F:150:GLU:OE2	2:F:153:ARG:NH1	2.49	0.45
1:C:133:ASN:OD1	1:C:255:ARG:NH2	2.48	0.45
2:B:127:ARG:NH1	2:F:131:GLU:OE1	2.49	0.44
1:A:135:ARG:NH1	1:A:145:SER:O	2.50	0.44
1:E:133:ASN:OD1	1:E:255:ARG:NH2	2.49	0.44
1:E:321:ARG:HG2	1:E:321:ARG:NH1	2.27	0.44
1:A:77:ASP:O	1:A:80:GLN:HG3	2.18	0.44
1:C:200:GLY:HA3	1:C:250:ASN:OD1	2.17	0.44
1:E:283:THR:HG22	1:E:285:ASN:H	1.83	0.44
1:A:57:ARG:NH2	1:A:82:GLU:OE1	2.50	0.44
1:E:89:GLU:OE1	1:E:109:ARG:NH1	2.50	0.44
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.18	0.44
1:C:180:TRP:CH2	1:C:213:ILE:HD13	2.53	0.44
1:E:53:ASN:OD1	1:E:276:THR:HA	2.17	0.44
1:E:109:ARG:HD2	1:E:109:ARG:HH11	1.69	0.43
2:F:9:PHE:CD1	2:F:10:ILE:HG13	2.53	0.43
2:D:26:HIS:ND1	2:D:149:ILE:HG21	2.34	0.43
1:C:213:ILE:HG12	1:C:233:TYR:CZ	2.53	0.43
1:E:11:ALA:HB3	2:F:140:ILE:HB	2.01	0.43
1:C:15:LEU:HD22	2:D:119:PHE:HA	2.01	0.43
1:A:283:THR:HG22	1:A:285:ASN:H	1.83	0.43
1:A:283:THR:HG22	1:A:285:ASN:N	2.34	0.43
1:C:283:THR:HG22	1:C:285:ASN:N	2.33	0.43
2:D:127:ARG:HB3	2:D:128:GLU:H	1.64	0.43
1:A:321:ARG:NH1	1:A:321:ARG:HG2	2.29	0.43
2:F:128:GLU:HG3	2:F:170:ARG:HH21	1.84	0.42
1:E:180:TRP:CH2	1:E:213:ILE:HD13	2.54	0.42
2:D:143:LYS:NZ	2:D:145:ASP:HB3	2.34	0.42
2:D:26:HIS:CG	2:D:149:ILE:HG21	2.53	0.42
2:B:128:GLU:HG3	2:B:170:ARG:HH21	1.83	0.42
1:E:200:GLY:HA3	1:E:250:ASN:OD1	2.19	0.42
1:A:15:LEU:HD22	2:B:119:PHE:HA	2.00	0.42
2:B:25:ARG:HG2	2:B:34:GLN:HG3	2.01	0.42
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.54	0.42
1:C:321:ARG:NH1	1:C:321:ARG:HG2	2.29	0.42
1:E:284:PRO:HG2	1:E:298:ASN:ND2	2.35	0.42
1:E:326:LYS:HD2	1:E:327:GLN:N	2.35	0.42
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.42
1:E:47:SER:HA	1:E:288:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:14:CYS:HA	2:D:137:CYS:HA	2.02	0.42
1:E:17:HIS:CE1	6:E:358:HOH:H2	2.37	0.41
1:C:89:GLU:OE1	1:C:109:ARG:NH1	2.52	0.41
1:A:11:ALA:HB3	2:B:140:ILE:HB	2.02	0.41
1:E:213:ILE:HG12	1:E:233:TYR:CZ	2.55	0.41
2:B:25:ARG:HA	2:B:34:GLN:HA	2.02	0.41
1:A:259:LYS:HB2	1:A:259:LYS:NZ	2.35	0.41
2:F:143:LYS:NZ	2:F:145:ASP:HB3	2.35	0.41
1:A:151:LEU:O	1:A:255:ARG:NH1	2.53	0.41
2:B:126:LEU:HD21	2:B:152:ILE:HD13	2.03	0.41
1:A:47:SER:HA	1:A:288:ILE:HG22	2.01	0.41
1:E:283:THR:HG22	1:E:285:ASN:N	2.36	0.41
1:E:259:LYS:HB2	1:E:259:LYS:NZ	2.36	0.41
1:C:57:ARG:NH2	1:C:82:GLU:OE1	2.54	0.41
1:C:151:LEU:O	1:C:255:ARG:NH1	2.54	0.41
1:E:14:CYS:HA	2:F:137:CYS:HA	2.03	0.41
1:A:109:ARG:HH11	1:A:109:ARG:HD2	1.68	0.41
2:D:128:GLU:HG3	2:D:170:ARG:HH21	1.86	0.41
1:C:284:PRO:HG2	1:C:298:ASN:ND2	2.36	0.41
1:A:86:LEU:HD11	1:A:268:MET:HB2	2.03	0.41
1:E:29:ILE:HD13	1:E:29:ILE:HA	1.95	0.41
1:A:283:THR:HB	1:A:286:GLY:O	2.22	0.40
1:C:201:ARG:HH11	1:C:201:ARG:HD3	1.77	0.40
1:A:2:ASP:CG	1:A:3:LEU:H	2.24	0.40
2:F:126:LEU:HD21	2:F:152:ILE:HD13	2.02	0.40
1:C:47:SER:HA	1:C:288:ILE:HG22	2.02	0.40
2:B:24:PHE:CD1	2:B:153:ARG:HD3	2.55	0.40
1:C:268:MET:SD	1:C:284:PRO:HD3	2.62	0.40
1:A:230:ILE:HD13	1:A:230:ILE:HG21	1.86	0.40
1:C:230:ILE:HD13	1:C:230:ILE:HG21	1.85	0.40
1:C:28:THR:HG23	2:D:105:GLN:OE1	2.21	0.40
1:C:66:LEU:HD22	1:C:267:ILE:HD12	2.04	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%)	305 (94%)	16 (5%)	5 (2%)	15	30
1	C	326/328 (99%)	307 (94%)	15 (5%)	4 (1%)	19	39
1	E	326/328 (99%)	312 (96%)	12 (4%)	2 (1%)	33	63
2	B	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	14	26
2	D	173/175 (99%)	161 (93%)	8 (5%)	4 (2%)	10	17
2	F	173/175 (99%)	159 (92%)	10 (6%)	4 (2%)	10	17
All	All	1497/1509 (99%)	1404 (94%)	71 (5%)	22 (2%)	15	30

All (22) 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
2	B	172	GLN
1	C	62	ILE
2	D	172	GLN
1	E	62	ILE
2	F	172	GLN
1	A	22	ASN
1	C	4	PRO
1	C	22	ASN
2	D	174	LYS
1	E	22	ASN
2	F	174	LYS

### 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%)	267 (92%)	23 (8%)	18	34
1	C	290/290 (100%)	268 (92%)	22 (8%)	19	36
1	E	290/290 (100%)	262 (90%)	28 (10%)	12	22
2	B	149/149 (100%)	144 (97%)	5 (3%)	49	78
2	D	149/149 (100%)	143 (96%)	6 (4%)	42	73
2	F	149/149 (100%)	143 (96%)	6 (4%)	42	73
All	All	1317/1317 (100%)	1227 (93%)	90 (7%)	22	43

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	18	HIS
1	A	28	THR
1	A	34	ILE
1	A	37	THR
1	A	82	GLU
1	A	103	PRO
1	A	145	SER
1	A	150	ARG
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	321	ARG
1	A	324	PRO
1	A	326	LYS
2	B	87	THR
2	B	127	ARG
2	B	145	ASP
2	B	160	ASP

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Mol	Chain	Res	Type
2	B	170	ARG
1	C	8	ASN
1	C	18	HIS
1	C	28	THR
1	C	34	ILE
1	C	37	THR
1	C	103	PRO
1	C	145	SER
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
1	C	324	PRO
2	D	87	THR
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	28	THR
1	E	34	ILE
1	E	37	THR
1	E	82	GLU
1	E	103	PRO
1	E	141	ARG
1	E	145	SER
1	E	150	ARG
1	E	155	THR
1	E	159	SER

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Mol	Chain	Res	Type
1	E	160	THR
1	E	189	GLN
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	309	VAL
1	E	321	ARG
1	E	324	PRO
1	E	326	LYS
1	E	328	THR
2	F	11	GLU
2	F	87	THR
2	F	127	ARG
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	81	ASN
1	A	171	ASN
1	C	38	ASN
1	C	81	ASN
1	C	171	ASN
1	E	38	ASN
1	E	81	ASN
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 ⓘ

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	12,14,15	0.67	0	15,19,21	0.92	1 (6%)
4	NAG	A	340	4	12,14,15	0.74	0	15,19,21	1.42	3 (20%)
4	BMA	A	341	4	10,11,12	0.79	0	11,15,17	0.94	0
4	NAG	C	339	1,4	12,14,15	0.85	0	15,19,21	1.00	1 (6%)
4	NAG	C	340	4	12,14,15	0.50	0	15,19,21	1.34	2 (13%)
4	BMA	C	341	4	10,11,12	0.44	0	11,15,17	1.01	1 (9%)
4	NAG	E	339	1,4	12,14,15	0.88	0	15,19,21	0.89	1 (6%)
4	NAG	E	340	4	12,14,15	0.67	0	15,19,21	1.26	2 (13%)
4	BMA	E	341	4	10,11,12	0.69	0	11,15,17	1.42	2 (18%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	341	BMA	O5-C5-C6	3.22	110.36	106.98
4	C	340	NAG	C3-C2-N2	-3.02	107.17	111.76
4	A	340	NAG	C3-C2-N2	-2.99	107.20	111.76
4	C	339	NAG	C3-C2-N2	-2.88	107.37	111.76
4	A	339	NAG	C3-C2-N2	-2.74	107.58	111.76
4	E	340	NAG	C3-C2-N2	-2.73	107.61	111.76
4	A	340	NAG	O5-C5-C4	-2.54	107.42	110.65
4	E	341	BMA	O5-C5-C4	-2.52	107.45	110.65
4	E	339	NAG	C3-C2-N2	-2.52	107.92	111.76
4	C	341	BMA	C6-C5-C4	-2.44	107.10	113.00
4	E	340	NAG	O5-C5-C4	-2.34	107.68	110.65
4	C	340	NAG	O5-C5-C4	-2.30	107.74	110.65
4	A	340	NAG	C4-C3-C2	-2.15	106.06	111.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

15 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	0.78	1 (8%)	15,19,21	0.84	0
3	NAG	A	334	1	12,14,15	0.65	0	15,19,21	1.33	2 (13%)
3	NAG	A	348	1	12,14,15	0.66	0	15,19,21	1.30	4 (26%)
5	MNA	A	349	-	22,22,22	0.97	0	32,32,32	1.37	4 (12%)
3	NAG	B	401	2	12,14,15	0.68	0	15,19,21	1.06	1 (6%)
3	NAG	C	329	1	12,14,15	0.83	1 (8%)	15,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	334	1	12,14,15	0.75	0	15,19,21	1.40	2 (13%)
3	NAG	C	348	1	12,14,15	0.79	0	15,19,21	1.38	3 (20%)
5	MNA	C	349	-	22,22,22	0.79	0	32,32,32	1.31	4 (12%)
3	NAG	D	401	2	12,14,15	0.74	0	15,19,21	1.01	1 (6%)
3	NAG	E	329	1	12,14,15	0.74	0	15,19,21	0.85	0
3	NAG	E	334	1	12,14,15	0.68	0	15,19,21	1.30	2 (13%)
3	NAG	E	348	1	12,14,15	0.71	0	15,19,21	1.37	3 (20%)
5	MNA	E	349	-	22,22,22	0.85	1 (4%)	32,32,32	1.43	3 (9%)
3	NAG	F	401	2	12,14,15	0.74	0	15,19,21	1.01	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
5	MNA	A	349	-	-	0/23/41/41	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
5	MNA	C	349	-	-	0/23/41/41	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
5	MNA	E	349	-	-	0/23/41/41	0/1/1/1
3	NAG	F	401	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	329	NAG	C4-C5	2.35	1.58	1.53
5	E	349	MNA	C3-C2	2.33	1.55	1.52
3	A	329	NAG	C4-C5	2.16	1.57	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	349	MNA	O1B-C1-C2	3.54	120.39	113.33
5	A	349	MNA	O1B-C1-C2	3.38	120.07	113.33
3	C	334	NAG	O5-C5-C6	3.38	110.53	106.98
3	A	334	NAG	O5-C5-C6	3.25	110.39	106.98
5	E	349	MNA	O6-C2-C3	-3.19	106.46	111.24
3	E	334	NAG	O5-C5-C6	3.15	110.28	106.98
5	C	349	MNA	C2-O6-C6	2.86	119.00	113.99
5	C	349	MNA	O1B-C1-C2	2.83	118.97	113.33
5	A	349	MNA	C2-O6-C6	2.83	118.94	113.99
3	C	334	NAG	O5-C5-C4	-2.64	107.31	110.65
3	E	348	NAG	C3-C4-C5	-2.50	105.75	110.20
3	E	334	NAG	O5-C5-C4	-2.49	107.50	110.65
5	E	349	MNA	C2-O6-C6	2.45	118.27	113.99
3	C	348	NAG	O5-C5-C4	-2.36	107.65	110.65
5	C	349	MNA	O6-C2-C3	-2.35	107.71	111.24
3	E	348	NAG	O5-C5-C4	-2.35	107.67	110.65
3	A	348	NAG	C3-C4-C5	-2.34	106.02	110.20
3	A	334	NAG	O5-C5-C4	-2.31	107.72	110.65
3	C	348	NAG	C3-C4-C5	-2.24	106.21	110.20
3	C	348	NAG	C8-C7-N2	2.23	120.46	116.11
5	A	349	MNA	O6-C6-C7	-2.20	103.50	106.34
3	B	401	NAG	C3-C2-N2	-2.13	108.52	111.76
5	A	349	MNA	O6-C2-C3	-2.10	108.09	111.24
3	E	348	NAG	C8-C7-N2	2.09	120.20	116.11
3	A	348	NAG	O4-C4-C5	2.08	114.77	109.28
5	C	349	MNA	C4-C5-N5	-2.04	105.61	110.12
3	D	401	NAG	C3-C2-N2	-2.03	108.67	111.76
3	A	348	NAG	O5-C5-C4	-2.02	108.09	110.65
3	A	348	NAG	C8-C7-N2	2.02	120.06	116.11

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%)	-0.29	13 (3%) 36 32	7, 26, 51, 149	0
1	C	328/328 (100%)	-0.30	12 (3%) 39 35	8, 26, 52, 153	0
1	E	328/328 (100%)	-0.28	12 (3%) 39 35	7, 26, 51, 148	0
2	B	175/175 (100%)	-0.50	4 (2%) 57 54	3, 23, 54, 108	0
2	D	175/175 (100%)	-0.52	6 (3%) 43 39	3, 22, 54, 108	0
2	F	175/175 (100%)	-0.54	6 (3%) 43 39	3, 23, 54, 108	0
All	All	1509/1509 (100%)	-0.37	53 (3%) 42 38	3, 25, 54, 153	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	11.4
1	A	7	ASP	10.4
1	A	328	THR	10.2
2	B	175	GLY	9.4
1	A	3	LEU	8.7
1	E	4	PRO	8.6
1	C	6	ASN	8.5
1	A	327	GLN	8.3
1	C	3	LEU	8.3
2	F	175	GLY	8.3
1	E	5	GLY	8.2
1	A	2	ASP	8.1
1	A	4	PRO	8.1
1	E	2	ASP	7.8
1	E	6	ASN	7.6
1	A	8	ASN	7.5
2	D	175	GLY	7.1
1	C	5	GLY	7.1
1	A	6	ASN	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	3	LEU	7.0
1	C	7	ASP	6.9
1	E	1	GLN	6.7
2	D	173	ILE	6.5
1	C	8	ASN	6.3
1	C	328	THR	6.3
1	A	1	GLN	6.2
1	C	4	PRO	6.2
1	E	328	THR	6.1
1	E	7	ASP	6.0
1	C	2	ASP	5.8
1	E	8	ASN	5.2
1	C	1	GLN	5.2
2	F	173	ILE	5.0
1	E	327	GLN	4.9
2	B	174	LYS	4.8
2	B	173	ILE	4.6
2	D	174	LYS	4.4
2	F	174	LYS	4.3
1	A	326	LYS	4.0
2	B	58	LYS	3.4
2	F	172	GLN	3.4
1	C	143	PRO	2.4
2	D	58	LYS	2.3
1	C	327	GLN	2.3
2	D	143	LYS	2.2
2	F	58	LYS	2.1
1	A	222	TRP	2.1
1	E	9	SER	2.1
2	F	59	THR	2.0
2	D	57	GLU	2.0
1	C	158	GLY	2.0
1	E	22	ASN	2.0
1	A	9	SER	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
4	NAG	A	339	14/15	0.16	0.52	0,0,45,47	0
4	NAG	A	340	14/15	0.18	0.44	0,0,56,58	0
4	NAG	C	339	14/15	0.17	0.33	0,0,45,47	0
4	NAG	C	340	14/15	0.17	0.09	0,0,56,60	0
4	NAG	E	340	14/15	0.15	-0.43	0,0,56,60	0
4	NAG	E	339	14/15	0.14	-0.49	0,0,45,47	0
4	BMA	E	341	11/12	0.30	-	0,0,69,71	0
4	BMA	A	341	11/12	0.24	-	0,0,63,64	0
4	BMA	C	341	11/12	0.33	-	0,0,70,71	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(Å <sup>2</sup> )	Q<0.9
3	NAG	D	401	14/15	0.38	9.82	0,0,66,67	0
3	NAG	E	329	14/15	0.30	8.79	0,0,51,51	0
3	NAG	C	329	14/15	0.27	7.93	0,0,51,51	0
3	NAG	A	329	14/15	0.27	7.15	0,0,51,51	0
3	NAG	C	348	14/15	0.29	6.53	0,0,50,51	0
3	NAG	A	348	14/15	0.24	6.11	0,0,49,51	0
3	NAG	E	348	14/15	0.24	6.10	0,0,50,51	0
3	NAG	F	401	14/15	0.29	5.57	0,0,66,67	0
3	NAG	B	401	14/15	0.35	5.50	0,0,66,67	0
3	NAG	C	334	14/15	0.21	2.83	0,0,49,51	0
3	NAG	A	334	14/15	0.17	1.42	0,0,48,50	0
3	NAG	E	334	14/15	0.15	0.25	0,0,49,51	0
5	MNA	C	349	22/22	0.13	-0.38	0,36,40,41	0
5	MNA	A	349	22/22	0.12	-0.48	0,36,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MNA	E	349	22/22	0.11	-0.89	0,35,40,41	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.