



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:36 PM GMT

PDB ID : 1RD8  
Title : Crystal Structure of the 1918 Human H1 Hemagglutinin Precursor (HA0)  
Authors : Stevens, J.; Corper, A.L.; Basler, C.F.; Taubenberger, J.K.; Palese, P.; Wilson, I.A.  
Deposited on : 2003-11-05  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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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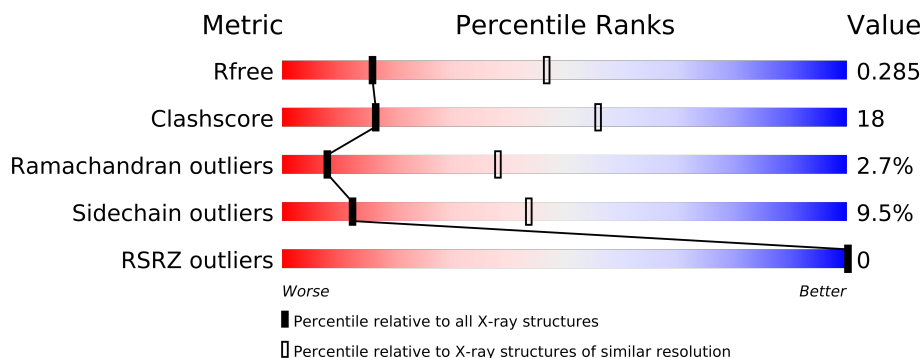
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	335	
1	C	335	
1	E	335	
2	B	182	
2	D	182	
2	F	182	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12082 atoms, of which 0 are hydrogen 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	23	0	0
			2549	1605	439	494	11			
1	C	328	Total	C	N	O	S	46	0	0
			2549	1605	439	494	11			
1	E	328	Total	C	N	O	S	44	0	0
			2549	1605	439	494	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	CLONING ARTIFACT	GB 4325039
A	4	ASP	-	CLONING ARTIFACT	GB 4325039
A	5	PRO	-	CLONING ARTIFACT	GB 4325039
A	6	GLY	-	CLONING ARTIFACT	GB 4325039
A	7	TYR	-	CLONING ARTIFACT	GB 4325039
A	8	LEU	-	CLONING ARTIFACT	GB 4325039
A	9	LEU	-	CLONING ARTIFACT	GB 4325039
A	10	GLU	-	CLONING ARTIFACT	GB 4325039
C	3	ALA	-	CLONING ARTIFACT	GB 4325039
C	4	ASP	-	CLONING ARTIFACT	GB 4325039
C	5	PRO	-	CLONING ARTIFACT	GB 4325039
C	6	GLY	-	CLONING ARTIFACT	GB 4325039
C	7	TYR	-	CLONING ARTIFACT	GB 4325039
C	8	LEU	-	CLONING ARTIFACT	GB 4325039
C	9	LEU	-	CLONING ARTIFACT	GB 4325039
C	10	GLU	-	CLONING ARTIFACT	GB 4325039
E	3	ALA	-	CLONING ARTIFACT	GB 4325039
E	4	ASP	-	CLONING ARTIFACT	GB 4325039
E	5	PRO	-	CLONING ARTIFACT	GB 4325039
E	6	GLY	-	CLONING ARTIFACT	GB 4325039
E	7	TYR	-	CLONING ARTIFACT	GB 4325039
E	8	LEU	-	CLONING ARTIFACT	GB 4325039
E	9	LEU	-	CLONING ARTIFACT	GB 4325039

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLU	-	CLONING ARTIFACT	GB 4325039

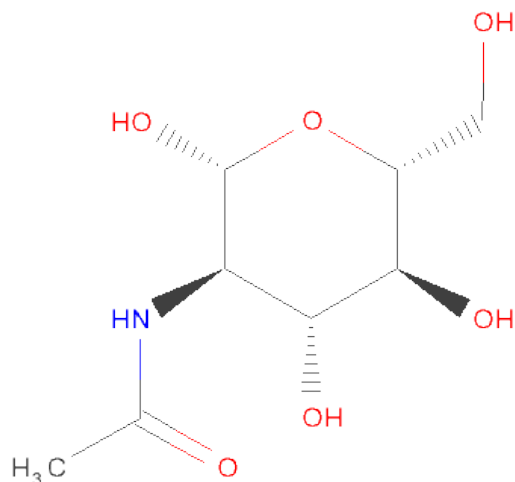
- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	16	0	0
			1406	877	241	282	6			
2	D	175	Total	C	N	O	S	29	0	0
			1406	877	241	282	6			
2	F	175	Total	C	N	O	S	35	0	0
			1406	877	241	282	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	LYS	CLONING ARTIFACT	GB 4325039
B	178	SER	-	CLONING ARTIFACT	GB 4325039
B	179	LEU	-	CLONING ARTIFACT	GB 4325039
B	180	VAL	-	CLONING ARTIFACT	GB 4325039
B	181	PRO	-	CLONING ARTIFACT	GB 4325039
B	182	ARG	-	CLONING ARTIFACT	GB 4325039
D	177	ARG	LYS	CLONING ARTIFACT	GB 4325039
D	178	SER	-	CLONING ARTIFACT	GB 4325039
D	179	LEU	-	CLONING ARTIFACT	GB 4325039
D	180	VAL	-	CLONING ARTIFACT	GB 4325039
D	181	PRO	-	CLONING ARTIFACT	GB 4325039
D	182	ARG	-	CLONING ARTIFACT	GB 4325039
F	177	ARG	LYS	CLONING ARTIFACT	GB 4325039
F	178	SER	-	CLONING ARTIFACT	GB 4325039
F	179	LEU	-	CLONING ARTIFACT	GB 4325039
F	180	VAL	-	CLONING ARTIFACT	GB 4325039
F	181	PRO	-	CLONING ARTIFACT	GB 4325039
F	182	ARG	-	CLONING ARTIFACT	GB 4325039

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	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	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	CLONING ARTIFACT	GB 4325039
A	4	ASP	-	CLONING ARTIFACT	GB 4325039
A	5	PRO	-	CLONING ARTIFACT	GB 4325039
A	6	GLY	-	CLONING ARTIFACT	GB 4325039
A	7	TYR	-	CLONING ARTIFACT	GB 4325039

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Chain	Residue	Modelled	Actual	Comment	Reference
A	8	LEU	-	CLONING ARTIFACT	GB 4325039
A	9	LEU	-	CLONING ARTIFACT	GB 4325039
A	10	GLU	-	CLONING ARTIFACT	GB 4325039
E	3	ALA	-	CLONING ARTIFACT	GB 4325039
E	4	ASP	-	CLONING ARTIFACT	GB 4325039
E	5	PRO	-	CLONING ARTIFACT	GB 4325039
E	6	GLY	-	CLONING ARTIFACT	GB 4325039
E	7	TYR	-	CLONING ARTIFACT	GB 4325039
E	8	LEU	-	CLONING ARTIFACT	GB 4325039
E	9	LEU	-	CLONING ARTIFACT	GB 4325039
E	10	GLU	-	CLONING ARTIFACT	GB 4325039

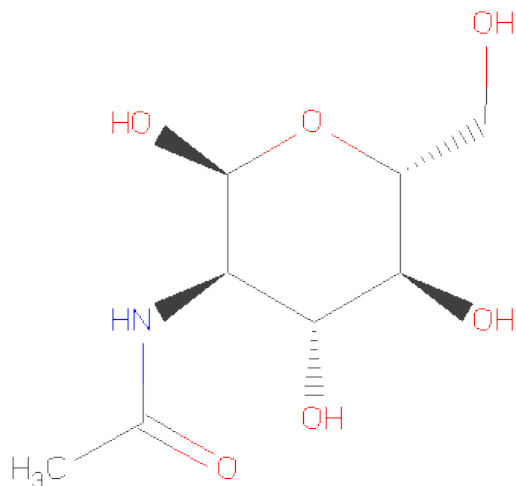
- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	4	Total	C	N	O	0	0
			50	28	2	20		

There are 8 discrepancies between the modelled and reference sequences:

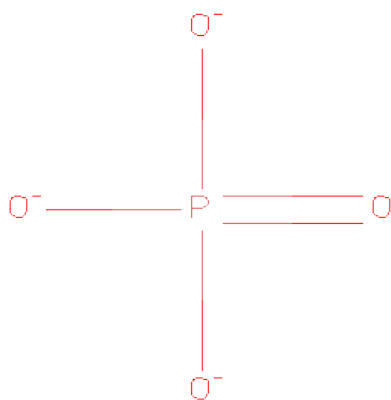
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ALA	-	CLONING ARTIFACT	GB 4325039
C	4	ASP	-	CLONING ARTIFACT	GB 4325039
C	5	PRO	-	CLONING ARTIFACT	GB 4325039
C	6	GLY	-	CLONING ARTIFACT	GB 4325039
C	7	TYR	-	CLONING ARTIFACT	GB 4325039
C	8	LEU	-	CLONING ARTIFACT	GB 4325039
C	9	LEU	-	CLONING ARTIFACT	GB 4325039
C	10	GLU	-	CLONING ARTIFACT	GB 4325039

- Molecule 6 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



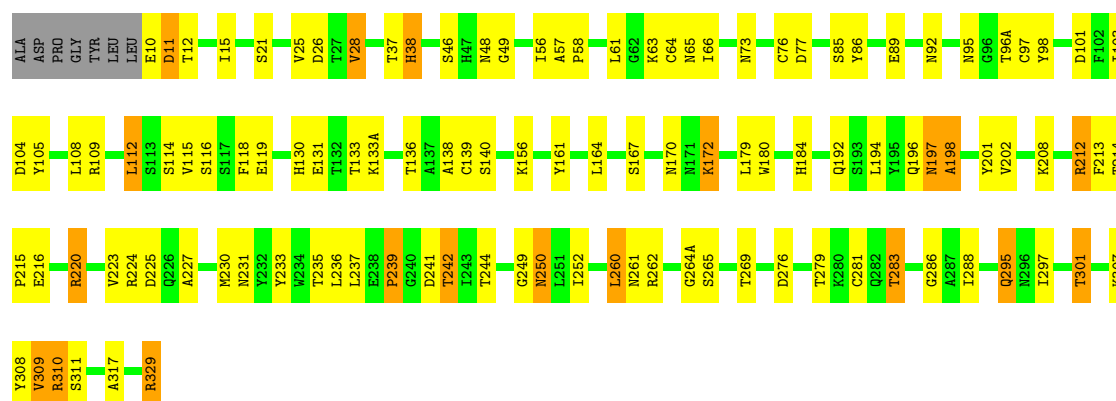
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	B	1	5	4	1	0	0

### 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.

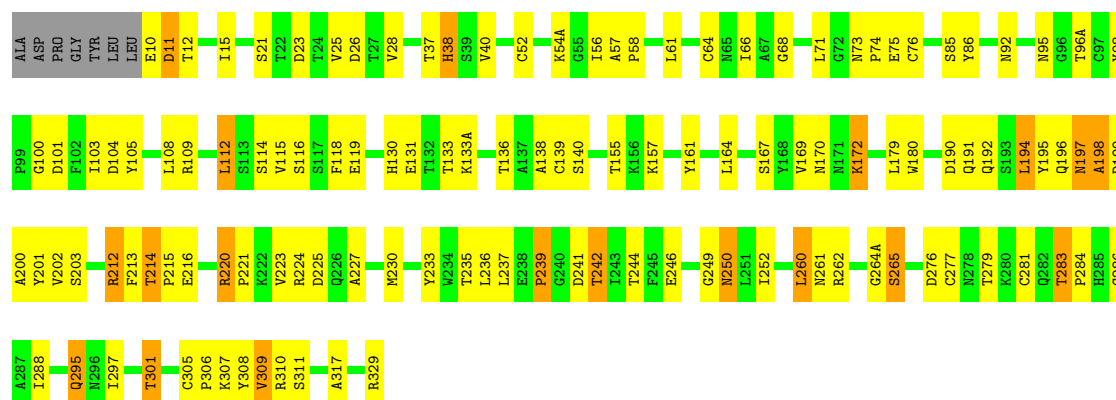
- Molecule 1: hemagglutinin

Chain A: 



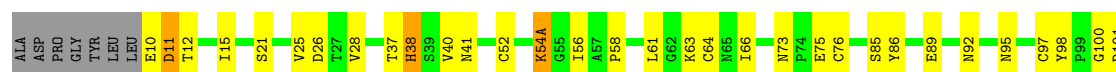
- Molecule 1: hemagglutinin

Chain C: 

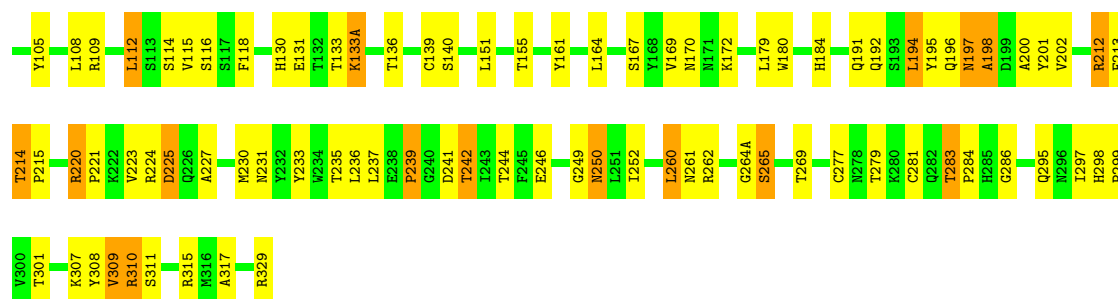


- Molecule 1: hemagglutinin

Chain E: 

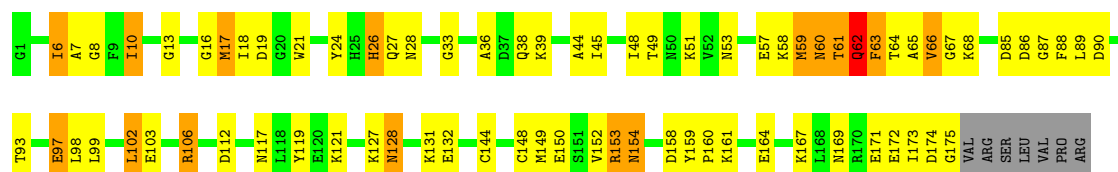






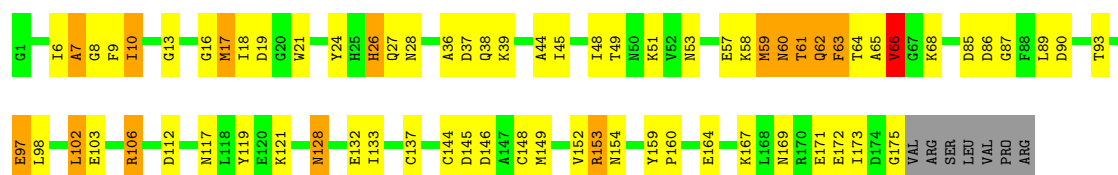
• Molecule 2: hemagglutinin

Chain B:



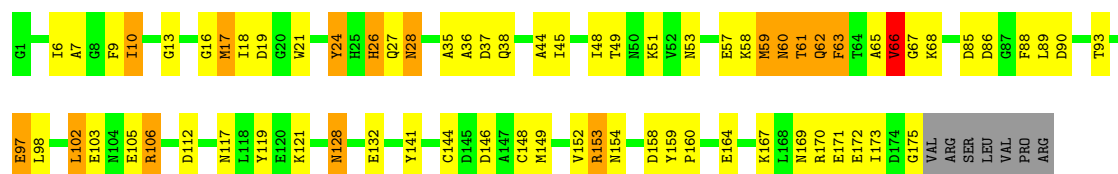
• Molecule 2: hemagglutinin

Chain D:



• Molecule 2: hemagglutinin

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.53Å 109.95Å 136.24Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 49.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-3.00) 96.1 (49.49-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.270 , 0.295 0.258 , 0.285	Depositor DCC
$R_{free}$ test set	2573 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 33.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 51346 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BMA, NAG, NDG, MAN

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	2/2613 (0.1%)	0.96	8/3558 (0.2%)
1	C	0.87	3/2613 (0.1%)	0.97	9/3558 (0.3%)
1	E	1.06	6/2613 (0.2%)	0.96	8/3558 (0.2%)
2	B	0.98	2/1433 (0.1%)	1.03	7/1929 (0.4%)
2	D	1.01	2/1433 (0.1%)	1.23	13/1929 (0.7%)
2	F	1.09	4/1433 (0.3%)	1.10	11/1929 (0.6%)
All	All	0.98	19/12138 (0.2%)	1.02	56/16461 (0.3%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	LYS	CD-CE	-20.71	0.99	1.51
1	E	133(A)	LYS	CG-CD	19.43	2.18	1.52
1	E	192	GLN	CA-CB	-9.37	1.33	1.53
2	F	175	GLY	N-CA	-9.17	1.32	1.46
1	C	133(A)	LYS	CA-CB	-8.69	1.34	1.53

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	PHE	CB-CG-CD2	-20.79	106.25	120.80
2	D	9	PHE	CB-CG-CD1	19.17	134.22	120.80
2	B	112	ASP	CB-CG-OD2	9.63	126.97	118.30
2	F	112	ASP	CB-CG-OD2	9.06	126.46	118.30
2	D	112	ASP	CB-CG-OD2	8.55	125.99	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	2549	0	2468	89	0
1	C	2549	0	2468	99	0
1	E	2549	0	2470	95	0
2	B	1406	0	1315	75	0
2	D	1406	0	1316	60	0
2	F	1406	0	1316	63	0
3	A	28	0	26	0	0
3	B	14	0	13	2	0
3	C	28	0	26	0	0
4	A	39	0	34	0	0
4	E	39	0	34	5	0
5	C	50	0	43	4	0
6	E	14	0	13	1	0
7	B	5	0	0	0	0
All	All	12082	0	11542	417	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 18.

The worst 5 of 417 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:106:ARG:HD3	2:F:106:ARG:HH12	1.34	0.90
2:B:106:ARG:HH12	2:D:106:ARG:HD3	1.36	0.89
2:D:106:ARG:HH12	2:F:106:ARG:HD3	1.37	0.88
2:B:117:ASN:HD21	2:B:121:LYS:HE2	1.37	0.88
1:A:15:ILE:HD11	2:B:119:TYR:HB2	1.55	0.88

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	326/335 (97%)	290 (89%)	33 (10%)	3 (1%)	25	73
1	C	326/335 (97%)	292 (90%)	31 (10%)	3 (1%)	25	73
1	E	326/335 (97%)	291 (89%)	32 (10%)	3 (1%)	25	73
2	B	173/182 (95%)	151 (87%)	12 (7%)	10 (6%)	3	15
2	D	173/182 (95%)	151 (87%)	11 (6%)	11 (6%)	2	11
2	F	173/182 (95%)	151 (87%)	12 (7%)	10 (6%)	3	15
All	All	1497/1551 (96%)	1326 (89%)	131 (9%)	40 (3%)	8	38

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA
2	B	10	ILE
2	B	60	ASN
2	B	62	GLN
2	B	66	VAL

### 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	284/289 (98%)	257 (90%)	27 (10%)	12	44
1	C	284/289 (98%)	258 (91%)	26 (9%)	13	46
1	E	284/289 (98%)	260 (92%)	24 (8%)	15	51
2	B	149/156 (96%)	133 (89%)	16 (11%)	10	35
2	D	149/156 (96%)	134 (90%)	15 (10%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	149/156 (96%)	134 (90%)	15 (10%)	11	39
All	All	1299/1335 (97%)	1176 (90%)	123 (10%)	12	44

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	214	THR
1	C	309	VAL
2	F	63	PHE
1	C	225	ASP
1	C	260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	196	GLN
2	D	27	GLN
2	F	30	GLN
1	C	231	ASN
1	C	275	HIS

### 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 ⓘ

10 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	330	1,4	12,14,15	0.93	1 (8%)	15,19,21	1.86	3 (20%)
4	NAG	A	331	4	12,14,15	0.74	0	15,19,21	2.12	3 (20%)
4	BMA	A	332	4	10,11,12	0.90	1 (10%)	11,15,17	2.65	2 (18%)
5	NAG	C	331	1,5	12,14,15	0.94	1 (8%)	15,19,21	1.31	2 (13%)
5	NAG	C	332	5	12,14,15	1.09	1 (8%)	15,19,21	1.94	5 (33%)
5	BMA	C	333	5	10,11,12	0.84	0	11,15,17	2.40	3 (27%)
5	MAN	C	334	5	10,11,12	0.63	0	11,15,17	2.29	3 (27%)
4	NAG	E	331	1,4	12,14,15	0.75	0	15,19,21	1.58	3 (20%)
4	NAG	E	332	4	12,14,15	0.87	0	15,19,21	2.35	4 (26%)
4	BMA	E	333	4	10,11,12	1.03	1 (10%)	11,15,17	1.61	3 (27%)

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	330	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	331	4	-	0/6/23/26	0/1/1/1
4	BMA	A	332	4	-	0/2/19/22	0/1/1/1
5	NAG	C	331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	332	5	-	0/6/23/26	0/1/1/1
5	BMA	C	333	5	-	0/2/19/22	0/1/1/1
5	MAN	C	334	5	-	0/2/19/22	0/1/1/1
4	NAG	E	331	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	332	4	-	0/6/23/26	0/1/1/1
4	BMA	E	333	4	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	333	BMA	O5-C5	-2.54	1.40	1.45
5	C	332	NAG	C2-N2	2.26	1.49	1.46
5	C	331	NAG	O5-C5	-2.20	1.41	1.45
4	A	332	BMA	O5-C5	-2.13	1.41	1.45
4	A	330	NAG	O3-C3	-2.02	1.38	1.43

The worst 5 of 31 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	332	BMA	O5-C5-C4	-6.53	102.36	110.65
5	C	334	MAN	O5-C5-C6	5.98	113.25	106.98
4	E	332	NAG	O5-C5-C6	5.90	113.17	106.98
4	A	332	BMA	O5-C5-C6	5.71	112.98	106.98
5	C	333	BMA	O5-C5-C6	5.53	112.78	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

7 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	1	1	12,14,15	0.86	1 (8%)	15,19,21	1.50	3 (20%)
3	NAG	A	2	1	12,14,15	0.62	0	15,19,21	1.33	1 (6%)
3	NAG	B	183	2	12,14,15	0.75	1 (8%)	15,19,21	1.61	3 (20%)
7	PO4	B	301	-	4,4,4	0.27	0	6,6,6	0.30	0
3	NAG	C	330	1	12,14,15	0.79	0	15,19,21	2.47	5 (33%)
3	NAG	C	335	1	12,14,15	0.88	0	15,19,21	2.17	3 (20%)
6	NDG	E	330	1	12,14,15	1.45	2 (16%)	15,19,21	2.77	8 (53%)

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	1	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	2	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	B	183	2	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PO4	B	301	-	-	0/0/0/0	0/0/0/0
3	NAG	C	330	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	335	1	-	2/6/23/26	0/1/1/1
6	NDG	E	330	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	330	NDG	C2-N2	3.17	1.50	1.46
6	E	330	NDG	C3-C2	2.52	1.57	1.52
3	A	1	NAG	C2-N2	2.03	1.48	1.46
3	B	183	NAG	O5-C5	-2.01	1.41	1.45

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	330	NAG	O5-C5-C4	-5.77	103.33	110.65
3	C	335	NAG	O5-C5-C4	-5.73	103.38	110.65
6	E	330	NDG	C3-C2-N2	5.58	120.26	111.76
3	C	335	NAG	O5-C5-C6	5.18	112.41	106.98
3	A	2	NAG	O5-C5-C6	4.64	111.85	106.98

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	NAG	C1
3	C	330	NAG	C1
3	B	183	NAG	C1
3	A	2	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	330	NDG	O7-C7-N2-C2
3	A	2	NAG	C8-C7-N2-C2
3	C	335	NAG	O7-C7-N2-C2
3	A	2	NAG	O7-C7-N2-C2
3	C	335	NAG	C8-C7-N2-C2

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	328/335 (97%)	-0.12	0 100 100	25, 42, 66, 97	6 (1%)
1	C	328/335 (97%)	-0.09	0 100 100	25, 42, 65, 97	13 (3%)
1	E	328/335 (97%)	-0.16	0 100 100	25, 42, 65, 97	14 (4%)
2	B	175/182 (96%)	-0.23	0 100 100	21, 36, 82, 108	4 (2%)
2	D	175/182 (96%)	-0.17	0 100 100	21, 36, 82, 108	7 (4%)
2	F	175/182 (96%)	-0.19	0 100 100	21, 36, 82, 108	10 (5%)
All	All	1509/1551 (97%)	-0.15	0 100 100	21, 40, 70, 108	54 (3%)

There are no RSRZ outliers to report.

### 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	BMA	C	333	11/12	0.28	-	78,81,85,89	0
4	BMA	E	333	11/12	0.35	-	83,85,89,89	0
4	NAG	E	332	14/15	0.32	-	64,70,73,79	0
5	NAG	C	331	14/15	0.21	-	45,48,54,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	331	14/15	0.37	-	71,77,82,89	0
4	NAG	A	330	14/15	0.19	-	44,45,53,62	0
5	MAN	C	334	11/12	0.59	-	93,95,98,99	0
4	BMA	A	332	11/12	0.39	-	91,96,97,98	0
5	NAG	C	332	14/15	0.38	-	76,84,88,89	0
4	NAG	E	331	14/15	0.19	-	41,47,53,56	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	C	335	14/15	0.41	-	90,95,95,96	0
7	PO4	B	301	5/5	0.24	-	61,62,63,64	0
3	NAG	A	1	14/15	0.39	-	71,75,78,78	0
3	NAG	C	330	14/15	0.45	-	71,76,78,78	0
3	NAG	B	183	14/15	0.39	-	74,82,84,86	0
6	NDG	E	330	14/15	0.28	-	63,66,70,71	0
3	NAG	A	2	14/15	0.32	-	70,78,79,81	0

## 6.5 Other polymers

There are no such residues in this entry.