



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 08:27 pm GMT

PDB ID : 1MQL  
Title : BHA of Ukr/63  
Authors : ha, y.; stevens, d.j.; shekel, j.j.; wiley, d.c.  
Deposited on : 2002-09-16  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

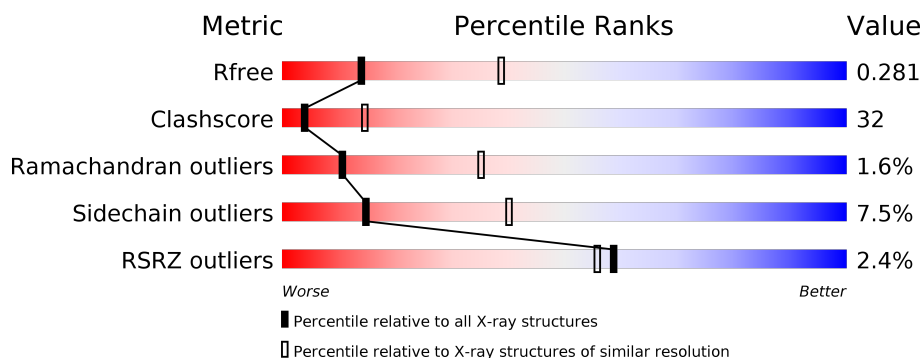
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	<div> <div>3%</div> <div> <div>43%</div> <div>48%</div> <div>6%</div> </div> </div>
1	D	329	<div> <div>%</div> <div> <div>52%</div> <div>40%</div> </div> </div>
1	G	329	<div> <div>2%</div> <div> <div>46%</div> <div>47%</div> </div> </div>
2	B	221	<div> <div>2%</div> <div> <div>45%</div> <div>29%</div> <div>22%</div> </div> </div>
2	E	221	<div> <div>%</div> <div> <div>41%</div> <div>32%</div> <div>5%</div> <div>22%</div> </div> </div>
2	H	221	<div> <div>2%</div> <div> <div>45%</div> <div>29%</div> <div>22%</div> </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	330	-	-	-	X
3	NAG	A	332	-	-	-	X
3	NAG	A	333	-	-	X	-
3	NAG	A	335	-	-	X	-
3	NAG	H	341	-	-	-	X
4	NDG	A	334	-	-	X	-
4	NDG	D	332	-	-	X	-
4	NDG	E	241	-	-	-	X
4	NDG	G	330	-	-	X	-
4	NDG	G	333	-	-	-	X
4	NDG	G	334	-	-	X	-
4	NDG	G	336	-	-	-	X
5	MAN	A	336	-	-	X	-
5	MAN	D	334	X	-	X	-
5	MAN	D	335	X	-	-	-
5	MAN	G	331	X	-	X	-
5	MAN	G	332	X	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2425	1522	424	466	13			
1	D	318	Total	C	N	O	S	0	0	0
			2432	1526	425	468	13			
1	G	318	Total	C	N	O	S	0	0	0
			2426	1523	424	466	13			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

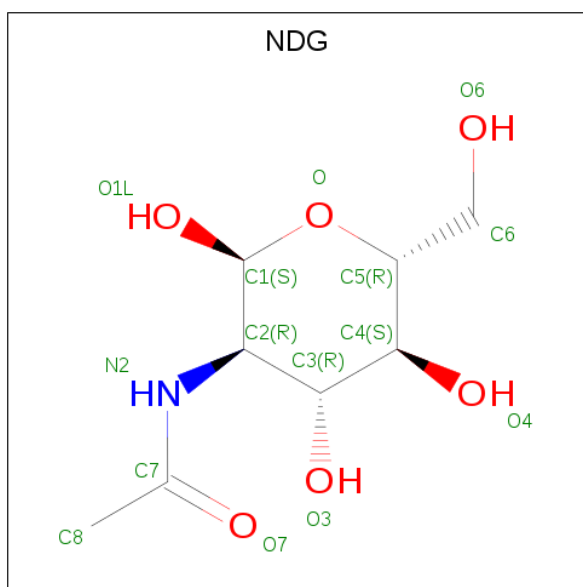
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1398	867	247	278	6			
2	E	172	Total	C	N	O	S	0	0	0
			1401	869	248	278	6			
2	H	172	Total	C	N	O	S	0	0	0
			1404	871	249	278	6			

- Molecule 3 is 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	N	O	0	0
			15	8	1	6		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			15	8	1	6		
3	G	1	Total	C	N	O	0	0
			15	8	1	6		
3	H	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 4 is 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
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		
4	E	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		
4	G	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		
5	A	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		
5	D	1	Total	C	O	0	0
			12	6	6		
5	G	1	Total	C	O	0	0
			12	6	6		
5	G	1	Total	C	O	0	0
			12	6	6		

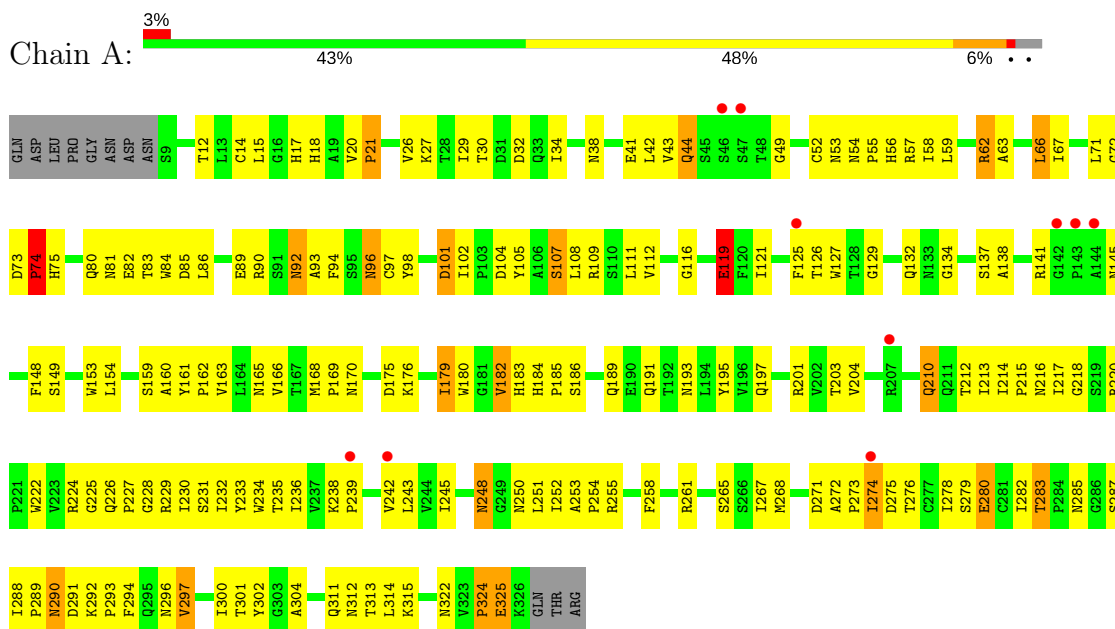
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	5	Total	O	0	0
			5	5		
6	D	11	Total	O	0	0
			11	11		
6	E	7	Total	O	0	0
			7	7		
6	G	9	Total	O	0	0
			9	9		
6	H	5	Total	O	0	0
			5	5		

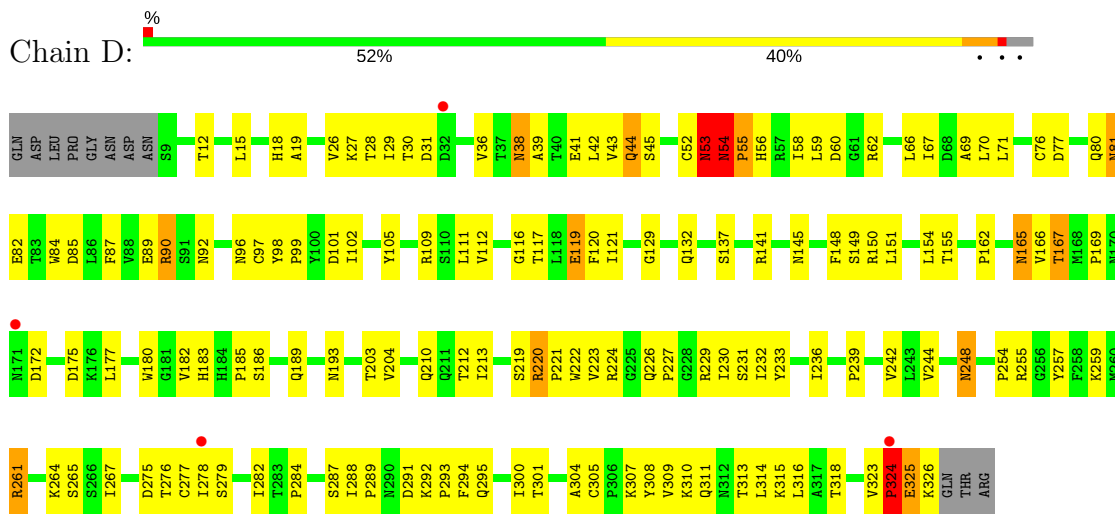
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Hemagglutinin HA1 chain

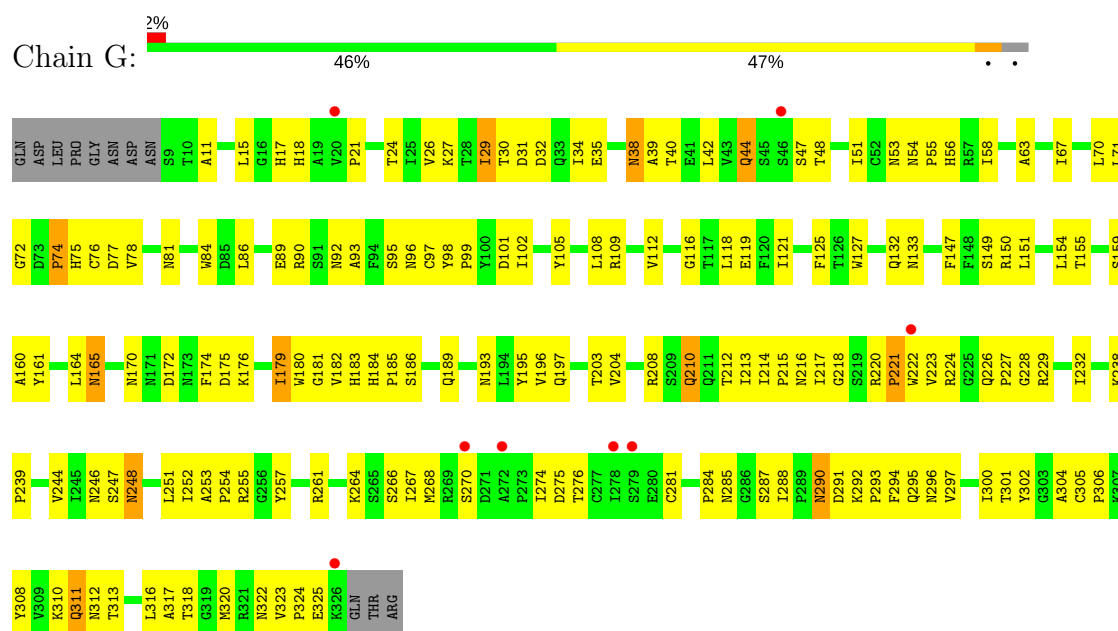


#### • Molecule 1: Hemagglutinin HA1 chain

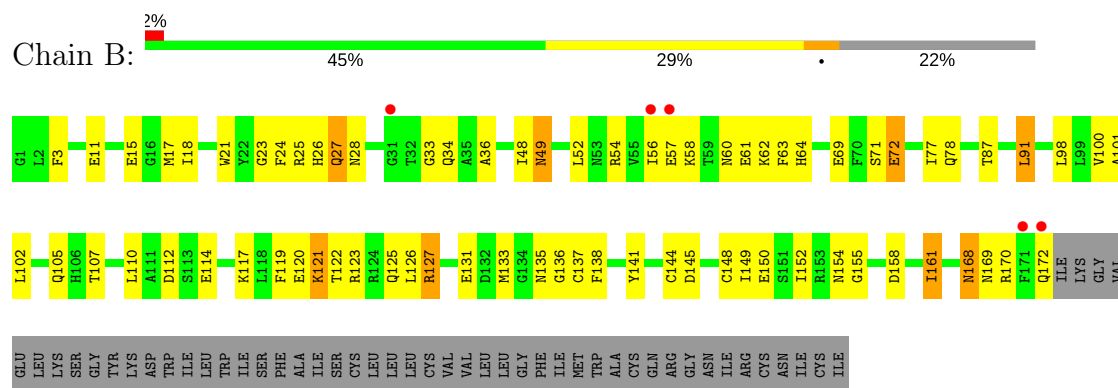


#### • Molecule 1: Hemagglutinin HA1 chain

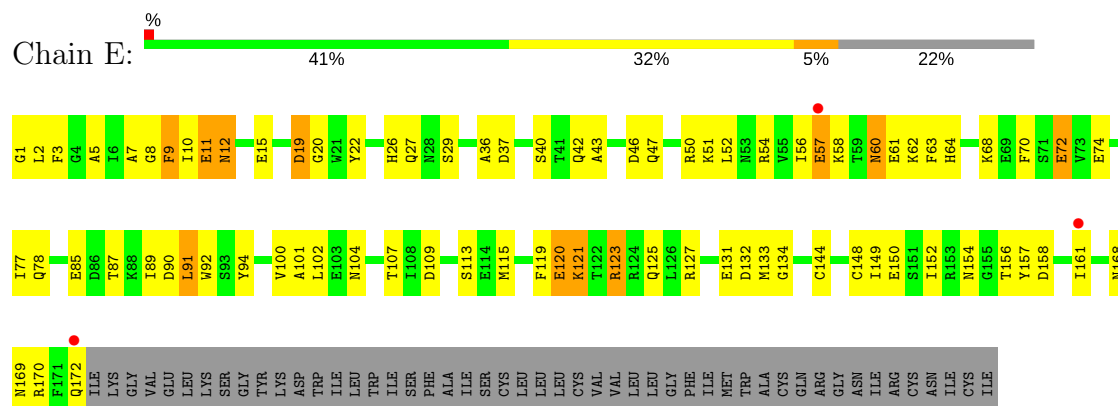




• Molecule 2: Hemagglutinin HA2 chain

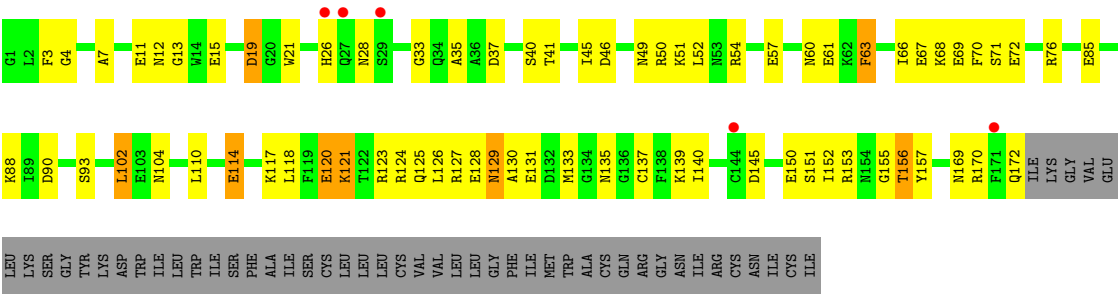


• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.68Å 147.10Å 251.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.15 – 2.91	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.90) 90.4 (40.15-2.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.269 , 0.306 0.245 , 0.281	Depositor DCC
$R_{free}$ test set	2979 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.45	1/2482 (0.0%)	0.68	0/3390
1	D	0.46	1/2489 (0.0%)	0.75	3/3398 (0.1%)
1	G	0.47	1/2483 (0.0%)	0.72	0/3391
2	B	0.45	0/1422	0.63	0/1912
2	E	0.42	0/1425	0.63	0/1915
2	H	0.40	0/1428	0.65	0/1918
All	All	0.45	3/11729 (0.0%)	0.69	3/15924 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	119	GLU	CB-CG	-5.29	1.42	1.52
1	D	119	GLU	CB-CG	-5.07	1.42	1.52
1	A	119	GLU	CB-CG	-5.07	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	ASN	N-CA-C	7.32	130.76	111.00
1	D	54	ASN	C-N-CD	6.18	141.37	128.40
1	D	53	ASN	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2425	0	2339	185	0
1	D	2432	0	2352	160	0
1	G	2426	0	2341	191	0
2	B	1398	0	1309	90	0
2	E	1401	0	1318	89	0
2	H	1404	0	1327	80	0
3	A	60	0	60	24	0
3	D	15	0	15	1	0
3	G	15	0	15	4	0
3	H	15	0	15	2	0
4	A	30	0	30	15	0
4	B	30	0	30	9	0
4	D	45	0	44	15	0
4	E	15	0	15	5	0
4	G	60	0	60	28	0
5	A	24	0	24	8	0
5	D	24	0	24	6	0
5	G	24	0	24	6	0
6	A	10	0	0	6	0
6	B	5	0	0	0	0
6	D	11	0	0	0	0
6	E	7	0	0	2	0
6	G	9	0	0	6	0
6	H	5	0	0	1	0
All	All	11890	0	11342	743	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 32.

The worst 5 of 743 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)
4:A:334:NDG:O4	4:B:222:NDG:H1	1.36	1.25
1:A:165:ASN:OD1	3:A:333:NAG:H1	1.40	1.19
2:B:125:GLN:HE22	2:B:155:GLY:HA2	1.09	1.18
4:D:333:NDG:H1	3:G:335:NAG:C4	1.81	1.10
4:D:333:NDG:O4	5:D:334:MAN:H1	1.51	1.10

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	316/329 (96%)	268 (85%)	40 (13%)	8 (2%)	6	23
1	D	316/329 (96%)	283 (90%)	30 (10%)	3 (1%)	19	52
1	G	316/329 (96%)	276 (87%)	35 (11%)	5 (2%)	11	35
2	B	170/221 (77%)	145 (85%)	24 (14%)	1 (1%)	27	61
2	E	170/221 (77%)	153 (90%)	13 (8%)	4 (2%)	6	25
2	H	170/221 (77%)	150 (88%)	18 (11%)	2 (1%)	14	43
All	All	1458/1650 (88%)	1275 (87%)	160 (11%)	23 (2%)	11	35

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO
1	A	325	GLU
1	D	324	PRO
1	D	325	GLU
1	G	133	ASN

### 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	268/288 (93%)	248 (92%)	20 (8%)	15	40
1	D	270/288 (94%)	247 (92%)	23 (8%)	12	34
1	G	268/288 (93%)	249 (93%)	19 (7%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	145/190 (76%)	135 (93%)	10 (7%)	17	44
2	E	146/190 (77%)	134 (92%)	12 (8%)	12	35
2	H	147/190 (77%)	138 (94%)	9 (6%)	20	51
All	All	1244/1434 (87%)	1151 (92%)	93 (8%)	15	40

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	ASN
1	D	324	PRO
2	H	49	ASN
1	D	167	THR
1	D	231	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	171	ASN
2	E	60	ASN
2	H	60	ASN
1	D	296	ASN
2	E	125	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

25 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	330	-	15,15,15	0.82	1 (6%)	21,21,21	2.39	4 (19%)
4	NDG	A	331	-	15,15,15	1.10	2 (13%)	21,21,21	0.99	1 (4%)
3	NAG	A	332	-	15,15,15	1.33	1 (6%)	21,21,21	2.39	2 (9%)
3	NAG	A	333	-	15,15,15	0.53	0	21,21,21	1.48	3 (14%)
4	NDG	A	334	-	15,15,15	0.76	1 (6%)	21,21,21	1.07	2 (9%)
3	NAG	A	335	-	15,15,15	0.68	0	21,21,21	1.92	5 (23%)
5	MAN	A	336	5	12,12,12	0.97	1 (8%)	17,17,17	0.64	0
5	MAN	A	337	5	12,12,12	0.65	0	17,17,17	0.92	0
4	NDG	B	222	-	15,15,15	0.59	0	21,21,21	0.85	0
4	NDG	B	223	-	15,15,15	0.60	0	21,21,21	0.72	0
4	NDG	D	330	-	15,15,15	0.80	0	21,21,21	0.86	0
3	NAG	D	331	-	15,15,15	0.58	0	21,21,21	1.66	3 (14%)
4	NDG	D	332	-	15,15,15	1.61	1 (6%)	21,21,21	1.77	5 (23%)
4	NDG	D	333	-	15,15,15	1.05	2 (13%)	21,21,21	1.23	3 (14%)
5	MAN	D	334	-	12,12,12	0.73	0	17,17,17	1.77	3 (17%)
5	MAN	D	335	-	12,12,12	0.51	0	17,17,17	0.47	0
4	NDG	E	241	-	15,15,15	0.49	0	21,21,21	0.58	0
4	NDG	G	330	-	15,15,15	0.81	1 (6%)	21,21,21	0.95	0
5	MAN	G	331	-	12,12,12	0.57	0	17,17,17	0.93	0
5	MAN	G	332	-	12,12,12	0.46	0	17,17,17	0.41	0
4	NDG	G	333	-	15,15,15	0.67	0	21,21,21	0.91	1 (4%)
4	NDG	G	334	-	15,15,15	0.66	0	21,21,21	0.86	1 (4%)
3	NAG	G	335	-	15,15,15	0.65	0	21,21,21	1.83	6 (28%)
4	NDG	G	336	-	15,15,15	0.69	0	21,21,21	0.77	0
3	NAG	H	341	-	15,15,15	0.46	0	21,21,21	1.28	1 (4%)

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	330	-	-	0/6/26/26	0/1/1/1
4	NDG	A	331	-	-	0/6/26/26	0/1/1/1
3	NAG	A	332	-	-	0/6/26/26	0/1/1/1
3	NAG	A	333	-	-	0/6/26/26	0/1/1/1
4	NDG	A	334	-	-	0/6/26/26	0/1/1/1
3	NAG	A	335	-	-	0/6/26/26	0/1/1/1
5	MAN	A	336	5	-	0/2/22/22	0/1/1/1
5	MAN	A	337	5	-	0/2/22/22	0/1/1/1
4	NDG	B	222	-	-	0/6/26/26	0/1/1/1
4	NDG	B	223	-	-	0/6/26/26	0/1/1/1
4	NDG	D	330	-	-	0/6/26/26	0/1/1/1
3	NAG	D	331	-	-	0/6/26/26	0/1/1/1
4	NDG	D	332	-	-	0/6/26/26	0/1/1/1
4	NDG	D	333	-	-	0/6/26/26	0/1/1/1
5	MAN	D	334	-	1/1/5/5	0/2/22/22	0/1/1/1
5	MAN	D	335	-	1/1/5/5	0/2/22/22	0/1/1/1
4	NDG	E	241	-	-	0/6/26/26	0/1/1/1
4	NDG	G	330	-	-	0/6/26/26	0/1/1/1
5	MAN	G	331	-	1/1/5/5	0/2/22/22	0/1/1/1
5	MAN	G	332	-	1/1/5/5	0/2/22/22	0/1/1/1
4	NDG	G	333	-	-	0/6/26/26	0/1/1/1
4	NDG	G	334	-	-	0/6/26/26	0/1/1/1
3	NAG	G	335	-	-	0/6/26/26	0/1/1/1
4	NDG	G	336	-	-	0/6/26/26	0/1/1/1
3	NAG	H	341	-	-	0/6/26/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	332	NDG	C1-C2	-5.51	1.46	1.52
4	D	333	NDG	C1-C2	-2.72	1.49	1.52
4	A	331	NDG	C1-C2	-2.19	1.50	1.52
5	A	336	MAN	C1-C2	-2.07	1.47	1.52
4	A	334	NDG	C1-C2	2.01	1.55	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	341	NAG	C1-C2-C3	-4.64	104.22	110.54
3	D	331	NAG	C1-C2-N2	-3.39	106.80	110.73
4	D	332	NDG	C1-C2-N2	-3.21	107.01	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	NAG	C1-C2-N2	-2.92	107.34	110.73
3	A	333	NAG	C1-C2-N2	-2.57	107.75	110.73

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	331	MAN	C1
5	D	335	MAN	C1
5	G	332	MAN	C1
5	D	334	MAN	C1

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	330	NAG	2	0
4	A	331	NDG	4	0
3	A	332	NAG	1	0
3	A	333	NAG	10	0
4	A	334	NDG	11	0
3	A	335	NAG	11	0
5	A	336	MAN	8	0
5	A	337	MAN	1	0
4	B	222	NDG	5	0
4	B	223	NDG	4	0
3	D	331	NAG	1	0
4	D	332	NDG	10	0
4	D	333	NDG	5	0
5	D	334	MAN	6	0
5	D	335	MAN	4	0
4	E	241	NDG	5	0
4	G	330	NDG	12	0
5	G	331	MAN	6	0
5	G	332	MAN	3	0
4	G	333	NDG	4	0
4	G	334	NDG	7	0
3	G	335	NAG	4	0
4	G	336	NDG	5	0
3	H	341	NAG	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	318/329 (96%)	0.14	10 (3%) 49 43	46, 71, 87, 98	0
1	D	318/329 (96%)	-0.06	4 (1%) 77 76	41, 59, 75, 95	0
1	G	318/329 (96%)	0.21	8 (2%) 57 54	47, 65, 82, 101	0
2	B	172/221 (77%)	0.06	5 (2%) 51 46	40, 64, 82, 100	0
2	E	172/221 (77%)	0.13	3 (1%) 70 69	41, 67, 85, 100	0
2	H	172/221 (77%)	0.26	5 (2%) 51 46	40, 66, 87, 101	0
All	All	1470/1650 (89%)	0.12	35 (2%) 59 56	40, 65, 84, 101	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	46	SER	4.7
2	B	57	GLU	4.3
2	H	27	GLN	4.1
2	H	29	SER	4.0
1	A	143	PRO	3.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	332	15/15	0.50	0.54	100,100,100,100	0
5	MAN	A	337	12/12	0.53	0.30	99,100,100,100	0
3	NAG	A	330	15/15	0.58	0.45	97,100,100,100	0
5	MAN	G	332	12/12	0.66	0.41	100,100,100,100	0
4	NDG	G	333	15/15	0.69	0.41	99,100,100,100	0
4	NDG	E	241	15/15	0.71	0.50	98,100,100,100	0
5	MAN	D	334	12/12	0.73	0.32	83,89,91,93	0
4	NDG	G	336	15/15	0.75	0.41	99,100,100,100	0
5	MAN	G	331	12/12	0.77	0.38	100,100,100,100	0
5	MAN	D	335	12/12	0.77	0.39	96,100,100,100	0
3	NAG	H	341	15/15	0.77	0.41	99,100,100,100	0
4	NDG	G	334	15/15	0.78	0.23	82,84,85,89	0
4	NDG	D	330	15/15	0.79	0.30	99,100,100,100	0
3	NAG	D	331	15/15	0.80	0.25	99,100,100,100	0
4	NDG	B	223	15/15	0.81	0.45	98,100,100,100	0
4	NDG	B	222	15/15	0.81	0.33	99,100,100,100	0
5	MAN	A	336	12/12	0.83	0.32	92,99,100,100	0
4	NDG	A	331	15/15	0.84	0.29	100,100,100,100	0
3	NAG	A	335	15/15	0.84	0.28	86,95,99,100	0
3	NAG	A	333	15/15	0.86	0.27	84,88,93,93	0
4	NDG	A	334	15/15	0.86	0.39	98,100,100,100	0
3	NAG	G	335	15/15	0.91	0.26	51,58,63,65	0
4	NDG	D	332	15/15	0.91	0.25	75,76,82,82	0
4	NDG	G	330	15/15	0.93	0.35	92,93,96,96	0
4	NDG	D	333	15/15	0.93	0.21	54,57,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.