



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:07 am GMT

PDB ID : 3ZP6  
Title : INFLUENZA VIRUS (VN1194) H5 E190D mutant HA with LSTc  
Authors : Liu, J.; Stevens, D.J.; Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2013-02-26  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

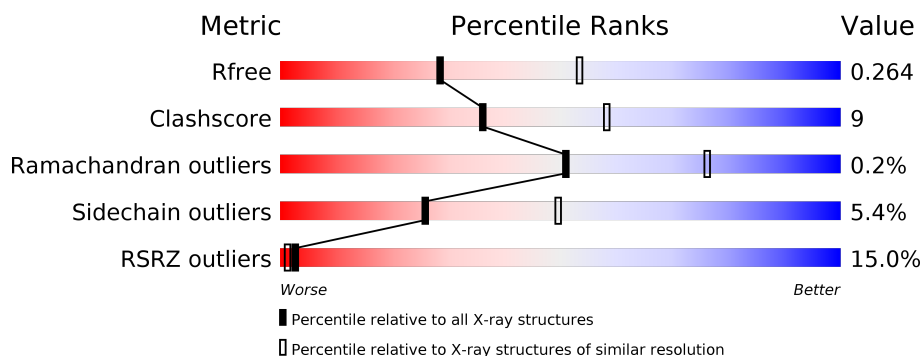
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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. 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	E	340	<div> <div>16%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• 6%</div> </div> </div>
2	F	160	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4007 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 HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	321	Total	C	N	O	S	0	0	0
			2548	1610	440	483	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	LYS	THR	CONFLICT	UNP Q6DQ34
E	190	ASP	GLU	ENGINEERED MUTATION	UNP Q6DQ34

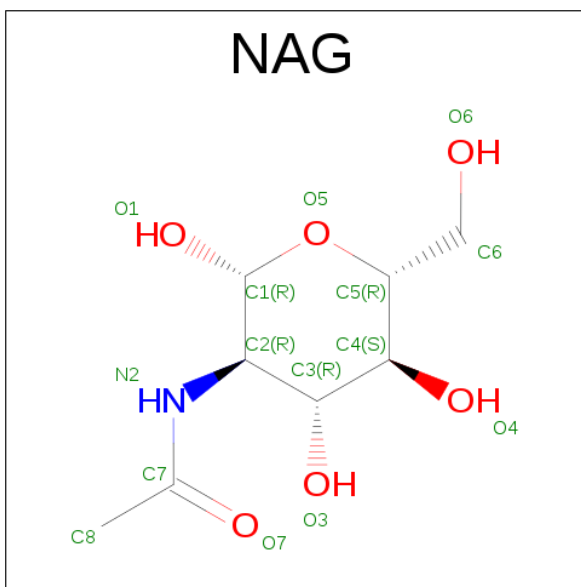
- Molecule 2 is a protein called HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	158	Total	C	N	O	S	0	0	0
			1272	791	221	252	8			

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 4 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
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

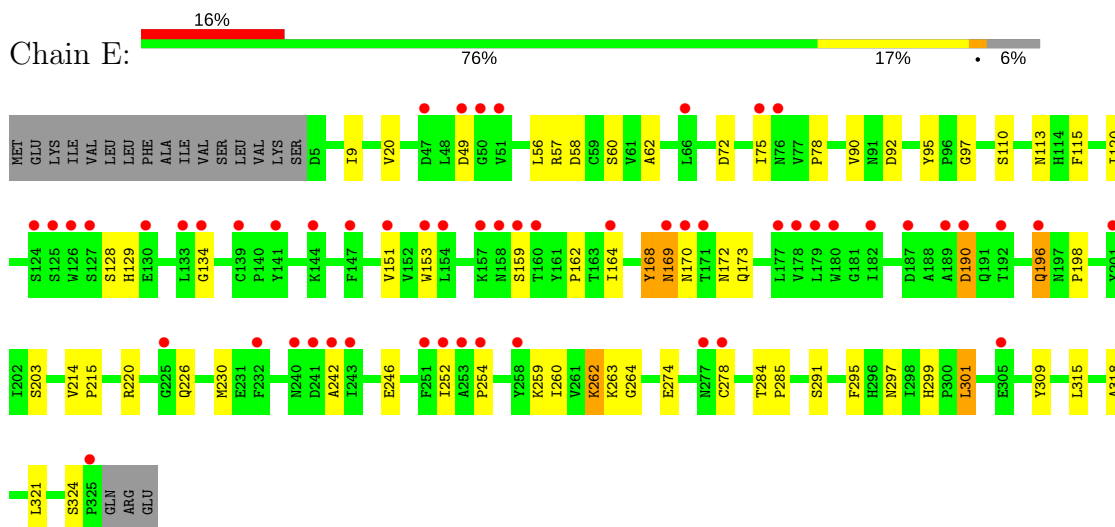
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	72	Total	O	0	0
			72	72		
5	F	62	Total	O	0	0
			62	62		

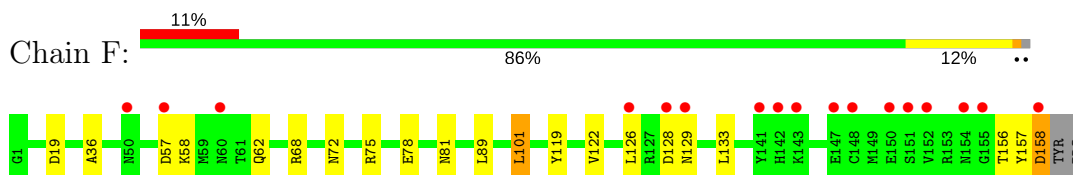
### 3 Residue-property plots [i](#)

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: HAEMAGGLUTININ



#### • Molecule 2: HAEMAGGLUTININ



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.39Å 101.39Å 450.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.95 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.60) 91.8 (29.95-2.52)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.223 , (Not available) 0.242 , 0.264	Depositor DCC
$R_{free}$ test set	1406 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: SIA, GAL, 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	E	0.38	0/2610	0.54	0/3545
2	F	0.45	0/1296	0.54	0/1742
All	All	0.40	0/3906	0.54	0/5287

There are no bond length outliers.

There are no bond angle outliers.

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	E	2548	0	2490	57	1
2	F	1272	0	1186	15	0
3	E	25	0	19	1	0
4	F	28	0	26	0	0
5	E	72	0	0	6	0
5	F	62	0	0	2	0
All	All	4007	0	3721	68	1

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 9.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:TYR:HD1	1:E:169:ASN:N	1.51	1.08
1:E:159:SER:O	1:E:196:GLN:OE1	1.83	0.97
1:E:57:ARG:O	5:E:2026:HOH:O	1.83	0.94
1:E:168:TYR:CD1	1:E:169:ASN:N	2.36	0.93
1:E:168:TYR:C	1:E:168:TYR:HD1	1.75	0.90
1:E:120:ILE:HG22	1:E:168:TYR:CE2	2.09	0.87
1:E:120:ILE:HG22	1:E:168:TYR:HE2	1.40	0.85
1:E:168:TYR:CE1	1:E:169:ASN:O	2.30	0.84
1:E:159:SER:C	1:E:196:GLN:OE1	2.17	0.83
1:E:168:TYR:HE1	1:E:169:ASN:O	1.62	0.81
1:E:299:HIS:HD2	1:E:301:LEU:H	1.30	0.80
1:E:168:TYR:CD1	1:E:168:TYR:C	2.51	0.79
2:F:19:ASP:HB3	2:F:36:ALA:HB2	1.66	0.78
1:E:72:ASP:O	1:E:75:ILE:HG12	1.86	0.76
1:E:110:SER:HB3	5:E:2042:HOH:O	1.84	0.75
1:E:60:SER:OG	1:E:92:ASP:OD1	2.04	0.75
1:E:128:SER:HB3	1:E:162:PRO:HG2	1.73	0.69
1:E:168:TYR:CE1	1:E:169:ASN:C	2.67	0.67
1:E:9:ILE:HD11	2:F:122:VAL:HG21	1.78	0.66
1:E:56:LEU:O	1:E:57:ARG:HB2	1.96	0.65
1:E:120:ILE:HB	1:E:168:TYR:HD2	1.62	0.65
1:E:92:ASP:O	5:E:2036:HOH:O	2.15	0.64
1:E:190:ASP:OD2	3:E:1326:SIA:H92	1.99	0.63
1:E:170:ASN:OD1	1:E:172:ASN:ND2	2.26	0.62
1:E:168:TYR:HE1	1:E:169:ASN:C	2.02	0.62
1:E:120:ILE:HB	1:E:168:TYR:CD2	2.35	0.61
1:E:169:ASN:OD1	1:E:169:ASN:C	2.39	0.60
1:E:299:HIS:CD2	1:E:301:LEU:H	2.18	0.59
1:E:113:ASN:OD1	1:E:264:GLY:HA3	2.03	0.57
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.87	0.57
1:E:168:TYR:HE1	1:E:170:ASN:HA	1.68	0.57
1:E:173:GLN:NE2	1:E:173:GLN:HA	2.21	0.55
1:E:120:ILE:CG2	1:E:168:TYR:CE2	2.87	0.55
2:F:157:TYR:O	2:F:158:ASP:HB2	2.07	0.55
2:F:156:THR:HG22	2:F:156:THR:O	2.08	0.54
1:E:115:PHE:HE1	1:E:260:ILE:HG12	1.72	0.54
1:E:95:TYR:CD1	1:E:230:MET:HG2	2.44	0.53
1:E:168:TYR:CE1	1:E:170:ASN:HA	2.44	0.52
1:E:151:VAL:HB	1:E:252:ILE:HG22	1.91	0.52
1:E:20:VAL:HG21	1:E:318:ALA:HB2	1.93	0.51
1:E:164:ILE:O	1:E:246:GLU:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:TYR:CD1	1:E:169:ASN:C	2.84	0.50
1:E:169:ASN:HA	1:E:242:ALA:HA	1.94	0.50
2:F:126:LEU:O	2:F:129:ASN:HB2	2.11	0.50
1:E:62:ALA:HB3	1:E:92:ASP:OD1	2.12	0.49
1:E:285:PRO:HD3	1:E:301:LEU:O	2.13	0.48
1:E:97:GLY:HA3	1:E:230:MET:O	2.14	0.48
1:E:309:TYR:HD2	2:F:89:LEU:HD22	1.77	0.48
1:E:58:ASP:HB3	1:E:90:VAL:HG22	1.94	0.48
2:F:19:ASP:HB2	5:F:2012:HOH:O	2.13	0.48
1:E:115:PHE:HE1	1:E:260:ILE:CG1	2.27	0.47
2:F:75:ARG:NH1	2:F:78:GLU:OE1	2.47	0.45
1:E:291:SER:HB2	5:E:2021:HOH:O	2.17	0.45
1:E:9:ILE:HG13	2:F:119:TYR:HA	1.98	0.45
1:E:120:ILE:HD11	1:E:254:PRO:HB2	2.00	0.44
1:E:129:HIS:HE1	5:E:2050:HOH:O	2.00	0.44
1:E:324:SER:HA	5:E:2069:HOH:O	2.18	0.44
2:F:72:ASN:HD22	2:F:75:ARG:HH21	1.65	0.44
1:E:203:SER:OG	1:E:246:GLU:HB3	2.18	0.43
1:E:169:ASN:HB2	1:E:242:ALA:HB2	2.00	0.43
2:F:72:ASN:ND2	2:F:75:ARG:HH21	2.17	0.43
2:F:101:LEU:HD13	5:F:2035:HOH:O	2.19	0.43
2:F:68:ARG:NH1	2:F:81:ASN:OD1	2.52	0.43
2:F:126:LEU:HD23	2:F:126:LEU:N	2.33	0.42
1:E:214:VAL:HA	1:E:215:PRO:HD3	1.88	0.41
1:E:115:PHE:CE1	1:E:260:ILE:HG12	2.54	0.41
1:E:168:TYR:HD1	1:E:169:ASN:CA	2.26	0.40
1:E:295:PHE:HE1	2:F:62:GLN:OE1	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LYS:NZ	1:E:262:LYS:NZ[11_565]	1.65	0.55

## 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	E	319/340 (94%)	306 (96%)	12 (4%)	1 (0%)	44	70
2	F	156/160 (98%)	153 (98%)	3 (2%)	0	100	100
All	All	475/500 (95%)	459 (97%)	15 (3%)	1 (0%)	51	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	198	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	289/307 (94%)	272 (94%)	17 (6%)	23	45
2	F	134/136 (98%)	128 (96%)	6 (4%)	32	59
All	All	423/443 (96%)	400 (95%)	23 (5%)	26	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	49	ASP
1	E	78	PRO
1	E	168	TYR
1	E	169	ASN
1	E	190	ASP
1	E	196	GLN
1	E	220	ARG
1	E	226	GLN
1	E	262	LYS
1	E	263	LYS
1	E	274	GLU

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Mol	Chain	Res	Type
1	E	278	CYS
1	E	284	THR
1	E	297	ASN
1	E	301	LEU
1	E	315	LEU
1	E	321	LEU
2	F	57	ASP
2	F	58	LYS
2	F	101	LEU
2	F	128	ASP
2	F	133	LEU
2	F	158	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	19	GLN
1	E	173	GLN
1	E	226	GLN
1	E	297	ASN
1	E	299	HIS
2	F	26	HIS
2	F	62	GLN
2	F	72	ASN
2	F	125	GLN
2	F	146	ASN
2	F	154	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 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	$\# Z  > 2$
3	SIA	E	1326	3	17,20,21	0.45	0	19,28,31	0.81	0
3	GAL	E	1327	3	4,4,12	0.34	0	2,4,17	1.23	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	SIA	E	1326	3	-	0/14/34/38	0/1/1/1
3	GAL	E	1327	3	-	0/2/2/22	0/0/0/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1326	SIA	1	0

## 5.6 Ligand geometry

2 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
4	NAG	F	411	1	14,14,15	0.40	0	15,19,21	0.56	0
4	NAG	F	421	1	14,14,15	0.44	0	15,19,21	1.09	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	411	1	-	0/6/23/26	0/1/1/1
4	NAG	F	421	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	421	NAG	C4-C3-C2	-2.02	108.06	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	E	321/340 (94%)	0.96	55 (17%)	2 1	26, 70, 95, 100	0
2	F	158/160 (98%)	0.55	17 (10%)	6 4	15, 45, 71, 95	0
All	All	479/500 (95%)	0.83	72 (15%)	3 1	15, 61, 93, 100	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	THR	7.3
1	E	158	ASN	7.3
2	F	148	CYS	5.4
1	E	160	THR	5.0
1	E	189	ALA	4.8
2	F	142	HIS	4.7
2	F	60	ASN	4.6
2	F	151	SER	4.6
1	E	171	THR	4.3
1	E	75	ILE	4.2
1	E	251	PHE	4.2
2	F	154	ASN	4.0
1	E	159	SER	3.8
2	F	158	ASP	3.8
1	E	252	ILE	3.8
2	F	57	ASP	3.7
1	E	190	ASP	3.7
1	E	66	LEU	3.7
1	E	125	SER	3.6
1	E	179	LEU	3.5
1	E	325	PRO	3.5
2	F	155	GLY	3.2
2	F	147	GLU	3.2
1	E	49	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	50	GLY	3.0
1	E	134	GLY	3.0
1	E	242	ALA	2.9
1	E	51	VAL	2.9
2	F	129	ASN	2.9
1	E	178	VAL	2.8
1	E	254	PRO	2.8
1	E	187	ASP	2.8
1	E	241	ASP	2.7
1	E	127	SER	2.7
2	F	128	ASP	2.7
1	E	164	ILE	2.7
1	E	157	LYS	2.7
1	E	278	CYS	2.7
1	E	305	GLU	2.7
1	E	133	LEU	2.7
1	E	147	PHE	2.7
2	F	143	LYS	2.7
1	E	76	ASN	2.7
1	E	47	ASP	2.6
1	E	253	ALA	2.6
1	E	169	ASN	2.6
1	E	141	TYR	2.6
1	E	177	LEU	2.6
1	E	130	GLU	2.6
1	E	151	VAL	2.5
2	F	150	GLU	2.5
1	E	124	SER	2.5
1	E	170	ASN	2.5
1	E	126	TRP	2.5
1	E	201	TYR	2.5
1	E	153	TRP	2.4
1	E	154	LEU	2.3
1	E	144	LYS	2.3
1	E	196	GLN	2.3
1	E	258	TYR	2.3
2	F	141	TYR	2.3
1	E	182	ILE	2.3
1	E	243	ILE	2.2
1	E	240	ASN	2.2
1	E	225	GLY	2.2
2	F	152	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	139	CYS	2.2
1	E	277	ASN	2.1
1	E	232	PHE	2.1
2	F	126	LEU	2.1
1	E	180	TRP	2.1
2	F	50	ASN	2.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SIA	E	1326	20/21	0.67	0.33	0.83	130,130,130,130	0
3	GAL	E	1327	5/12	0.51	0.32	-	130,130,131,131	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	F	421	14/15	0.80	0.38	0.87	73,73,74,74	0
4	NAG	F	411	14/15	0.82	0.48	-	79,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.