



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 03:43 AM EDT

PDB ID : 5VJL  
Title : Crystal structure of H7 hemagglutinin mutant (V186K, K193T, G228S) from the influenza virus A/Shanghai/2/2013 (H7N9) with LSTc  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2017-04-19  
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

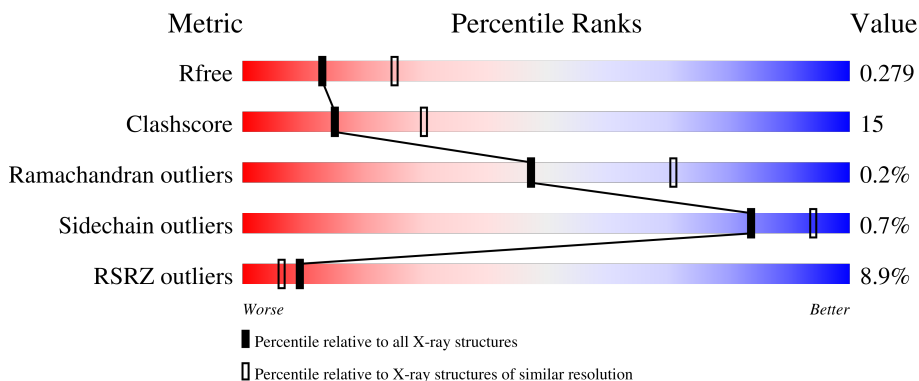
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	325	
2	B	183	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3852 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2397	1488	433	461	15	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP R4NN21
A	8	ASP	-	expression tag	UNP R4NN21
A	9	PRO	-	expression tag	UNP R4NN21
A	10	GLY	-	expression tag	UNP R4NN21
A	186	LYS	VAL	engineered mutation	UNP R4NN21
A	193	THR	LYS	engineered mutation	UNP R4NN21
A	228	SER	GLY	engineered mutation	UNP R4NN21

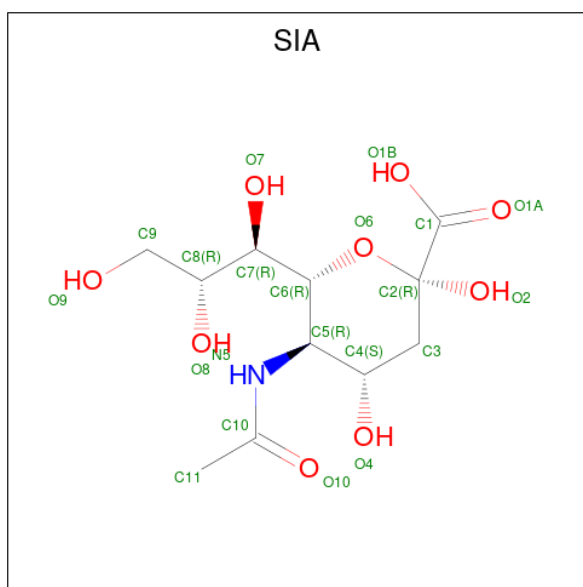
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	168	1360	841	235	277	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

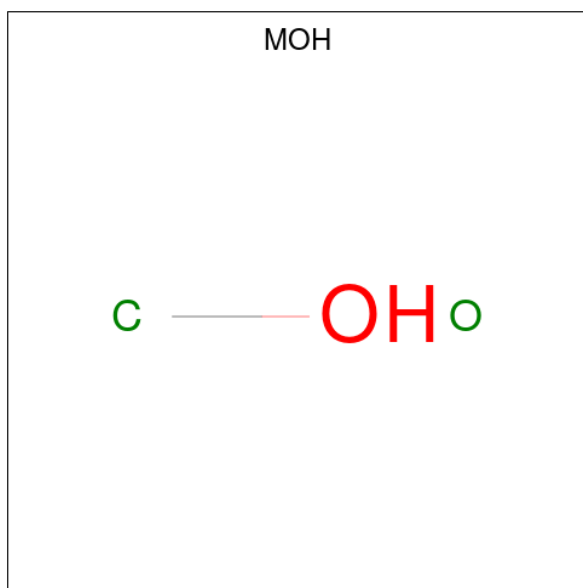
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP R4NN21
B	178	GLY	-	expression tag	UNP R4NN21
B	179	ARG	-	expression tag	UNP R4NN21
B	180	LEU	-	expression tag	UNP R4NN21
B	181	VAL	-	expression tag	UNP R4NN21
B	182	PRO	-	expression tag	UNP R4NN21
B	183	ARG	-	expression tag	UNP R4NN21

- Molecule 3 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	20	11	1	8	0	0

- Molecule 4 is METHANOL (three-letter code: MOH) (formula: CH<sub>4</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	2	1	1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0

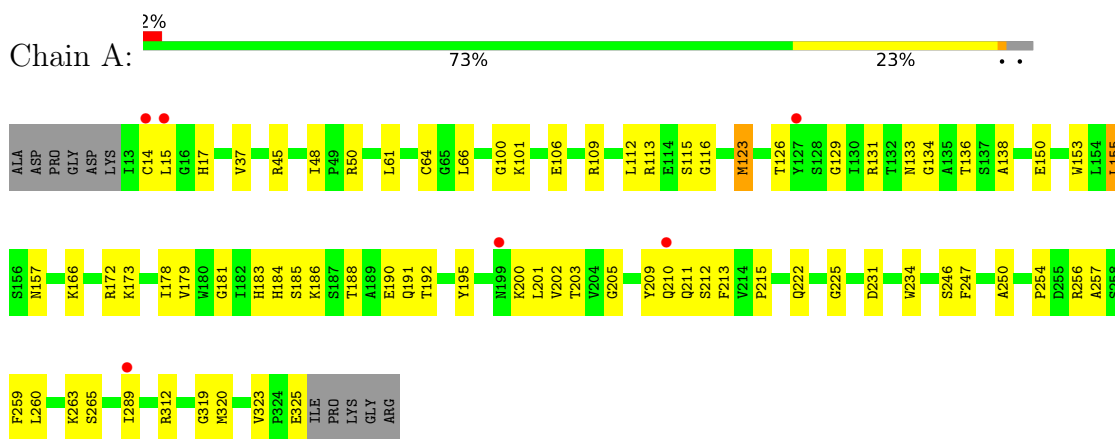
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	14	14	14	0	0
6	B	17	17	17	0	0

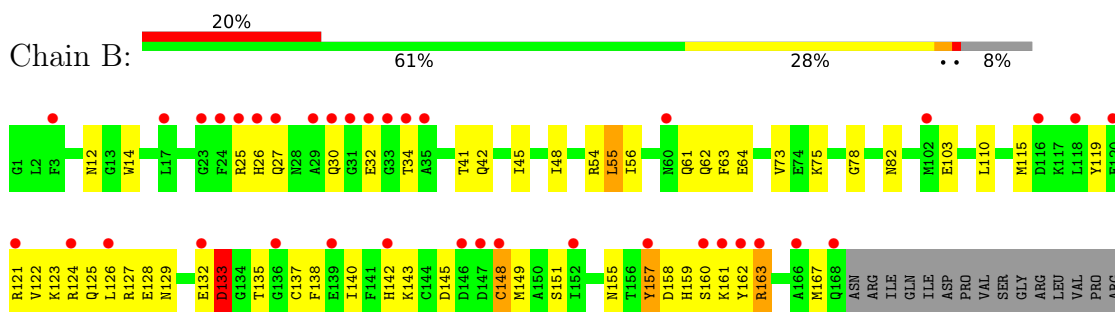
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



- Molecule 2: Hemagglutinin HA2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.38Å 116.38Å 296.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.70 – 2.60 47.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.70-2.60) 99.3 (47.70-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.218 , 0.277 0.218 , 0.279	Depositor DCC
$R_{free}$ test set	1232 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.5	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.020 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.006 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, MOH, 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	0.56	0/2443	0.82	2/3303 (0.1%)
2	B	0.63	1/1384 (0.1%)	1.09	7/1865 (0.4%)
All	All	0.58	1/3827 (0.0%)	0.93	9/5168 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	148	CYS	CB-SG	-6.30	1.71	1.82

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	LEU	CA-CB-CG	-9.56	93.31	115.30
2	B	163	ARG	CA-CB-CG	7.45	129.78	113.40
2	B	157	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	155	LEU	CB-CG-CD1	-6.63	99.72	111.00
2	B	124	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	B	124	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	66	LEU	CB-CG-CD2	-5.35	101.90	111.00
2	B	157	TYR	CB-CG-CD1	5.26	124.15	121.00
2	B	133	ASP	CB-CG-OD2	-5.20	113.62	118.30

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	2397	0	2352	57	0
2	B	1360	0	1261	61	0
3	A	20	0	17	1	0
4	A	2	0	0	0	0
5	A	28	0	26	0	0
5	B	14	0	13	3	0
6	A	14	0	0	2	0
6	B	17	0	0	2	0
All	All	3852	0	3669	112	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 15.

All (112) 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)
2:B:142:HIS:CE1	2:B:162:TYR:CD2	2.22	1.26
2:B:142:HIS:HE1	2:B:162:TYR:CE2	1.74	1.04
1:A:136:THR:HG22	1:A:138:ALA:H	1.22	0.98
2:B:142:HIS:HE1	2:B:162:TYR:CD2	1.68	0.97
2:B:140:ILE:HD13	2:B:143:LYS:HG2	1.52	0.92
2:B:140:ILE:HD12	2:B:140:ILE:O	1.76	0.85
2:B:142:HIS:CE1	2:B:162:TYR:CG	2.66	0.84
2:B:27:GLN:HB3	2:B:32:GLU:HG2	1.61	0.83
1:A:17:HIS:HB3	2:B:115:MET:HE2	1.62	0.81
2:B:142:HIS:ND1	2:B:162:TYR:CD2	2.49	0.80
2:B:126:LEU:HD12	2:B:138:PHE:HD2	1.47	0.80
2:B:140:ILE:CD1	2:B:143:LYS:HE3	2.12	0.78
1:A:45:ARG:HD3	1:A:312:ARG:HG3	1.66	0.77
1:A:173:LYS:O	1:A:173:LYS:HD2	1.84	0.76
2:B:25:ARG:HE	2:B:34:THR:HG21	1.48	0.75
1:A:123:MET:HE1	1:A:178:ILE:HD12	1.68	0.75
1:A:126:THR:O	1:A:166:LYS:NZ	2.24	0.71
2:B:133:ASP:OD2	2:B:135:THR:HB	1.90	0.70
1:A:48:ILE:HD12	1:A:289:ILE:HD12	1.74	0.69
2:B:142:HIS:CE1	2:B:162:TYR:CE2	2.63	0.68
2:B:75:LYS:HD2	5:B:201:NAG:H81	1.75	0.67
1:A:184:HIS:NE2	1:A:231:ASP:OD2	2.24	0.67
2:B:127:ARG:HH11	2:B:159:HIS:CE1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:THR:O	1:A:192:THR:HG23	1.94	0.67
1:A:209:TYR:CZ	1:A:211:GLN:HG3	2.30	0.66
1:A:17:HIS:HE1	1:A:323:VAL:HG12	1.61	0.66
2:B:140:ILE:CD1	2:B:143:LYS:HG2	2.26	0.65
1:A:201:LEU:HD11	1:A:212:SER:HB3	1.79	0.64
2:B:140:ILE:HD11	2:B:143:LYS:HE3	1.80	0.63
1:A:100:GLY:O	1:A:101:LYS:HD3	1.99	0.62
1:A:116:GLY:HA2	1:A:265:SER:HB3	1.81	0.62
1:A:222:GLN:OE1	1:A:225:GLY:HA2	2.02	0.60
2:B:26:HIS:HB2	2:B:149:MET:SD	2.42	0.60
2:B:160:SER:HA	2:B:163:ARG:HB2	1.84	0.59
1:A:37:VAL:HG22	1:A:319:GLY:HA3	1.84	0.58
1:A:179:VAL:O	1:A:254:PRO:HB3	2.04	0.58
2:B:128:GLU:O	2:B:128:GLU:HG3	2.03	0.58
1:A:210:GLN:O	1:A:211:GLN:HG2	2.04	0.57
2:B:129:ASN:ND2	2:B:159:HIS:O	2.37	0.56
2:B:158:ASP:OD2	2:B:161:LYS:HG2	2.06	0.56
2:B:140:ILE:O	2:B:140:ILE:CD1	2.53	0.55
2:B:56:ILE:HD12	2:B:56:ILE:O	2.07	0.54
1:A:179:VAL:HG22	1:A:234:TRP:HB3	1.89	0.54
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.07	0.54
1:A:200:LYS:O	1:A:215:PRO:HD2	2.07	0.53
2:B:119:TYR:CE1	2:B:138:PHE:HE1	2.26	0.53
2:B:82:ASN:OD1	5:B:201:NAG:H2	2.09	0.52
2:B:142:HIS:ND1	2:B:162:TYR:CG	2.76	0.52
1:A:123:MET:HE2	1:A:257:ALA:HB2	1.92	0.52
1:A:201:LEU:HD12	1:A:213:PHE:O	2.09	0.52
1:A:109:ARG:O	1:A:113:ARG:HG3	2.10	0.52
1:A:131:ARG:HB3	1:A:155:LEU:HD11	1.92	0.52
1:A:185:SER:OG	1:A:191:GLN:HB2	2.10	0.51
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.90	0.51
1:A:131:ARG:CZ	1:A:155:LEU:HD11	2.41	0.51
1:A:263:LYS:NZ	2:B:64:GLU:OE2	2.43	0.51
1:A:325:GLU:HA	2:B:12:ASN:ND2	2.26	0.51
1:A:136:THR:HG22	1:A:138:ALA:N	2.07	0.51
2:B:61:GLN:HG2	2:B:63:PHE:CE2	2.46	0.51
1:A:186:LYS:HD3	1:A:190:GLU:OE2	2.10	0.51
2:B:73:VAL:HG23	6:B:309:HOH:O	2.10	0.51
2:B:123:LYS:N	2:B:138:PHE:HE2	2.09	0.50
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.44	0.50
2:B:142:HIS:ND1	2:B:162:TYR:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA2	1:A:231:ASP:O	2.11	0.50
2:B:41:THR:O	2:B:45:ILE:HG23	2.12	0.50
2:B:121:ARG:O	2:B:125:GLN:HG3	2.12	0.50
2:B:157:TYR:CZ	2:B:159:HIS:HA	2.46	0.49
2:B:42:GLN:NE2	2:B:45:ILE:HD11	2.27	0.49
2:B:148:CYS:SG	2:B:162:TYR:HE2	2.34	0.49
2:B:123:LYS:HD2	2:B:132:GLU:OE1	2.11	0.49
2:B:25:ARG:HE	2:B:34:THR:CG2	2.21	0.48
1:A:100:GLY:C	1:A:101:LYS:HG2	2.34	0.48
2:B:127:ARG:NH1	2:B:159:HIS:CE1	2.82	0.48
1:A:14:CYS:HA	2:B:137:CYS:HA	1.96	0.48
1:A:123:MET:CE	1:A:257:ALA:HB2	2.44	0.48
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.96	0.47
2:B:62:GLN:NE2	2:B:64:GLU:OE2	2.48	0.47
2:B:142:HIS:CD2	2:B:143:LYS:N	2.82	0.47
2:B:128:GLU:O	2:B:128:GLU:CG	2.62	0.47
1:A:202:VAL:HA	1:A:246:SER:O	2.15	0.46
1:A:172:ARG:HD3	1:A:259:PHE:CZ	2.51	0.45
1:A:100:GLY:O	1:A:101:LYS:CD	2.63	0.45
1:A:210:GLN:C	1:A:211:GLN:HG2	2.37	0.45
1:A:323:VAL:HG13	1:A:323:VAL:O	2.16	0.45
2:B:54:ARG:HH22	2:B:103:GLU:CD	2.20	0.45
1:A:17:HIS:O	2:B:14:TRP:N	2.46	0.45
1:A:203:THR:HG23	6:A:3110:HOH:O	2.17	0.45
1:A:115:SER:HB2	1:A:260:LEU:HD22	1.99	0.45
1:A:195:TYR:CZ	1:A:250:ALA:HA	2.52	0.45
2:B:55:LEU:HA	2:B:55:LEU:HD23	1.57	0.44
2:B:125:GLN:NE2	2:B:155:ASN:CG	2.71	0.44
1:A:205:GLY:HA2	1:A:209:TYR:O	2.18	0.44
1:A:37:VAL:HG13	1:A:320:MET:O	2.18	0.44
1:A:202:VAL:HG22	1:A:247:PHE:CB	2.48	0.44
1:A:136:THR:HG23	3:A:3001:SIA:O1B	2.18	0.43
2:B:122:VAL:HG12	2:B:138:PHE:CE2	2.54	0.43
1:A:129:GLY:O	1:A:157:ASN:ND2	2.52	0.42
2:B:78:GLY:HA3	5:B:201:NAG:H82	2.00	0.42
2:B:163:ARG:HE	2:B:167:MET:HE1	1.84	0.42
1:A:131:ARG:HG2	1:A:133:ASN:OD1	2.20	0.42
2:B:161:LYS:N	2:B:161:LYS:HD3	2.32	0.42
1:A:106:GLU:OE1	6:A:3101:HOH:O	2.21	0.41
2:B:48:ILE:CD1	2:B:110:LEU:HD11	2.51	0.41
2:B:126:LEU:HD23	2:B:157:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:HIS:ND1	2:B:162:TYR:CB	2.84	0.41
2:B:142:HIS:CD2	2:B:143:LYS:H	2.39	0.41
1:A:184:HIS:CE1	1:A:215:PRO:HA	2.56	0.41
2:B:30:GLN:HE22	2:B:145:ASP:HA	1.87	0.40
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.78	0.40
2:B:73:VAL:HG12	6:B:306:HOH:O	2.21	0.40
1:A:61:LEU:HB3	1:A:64:CYS:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	312/325 (96%)	303 (97%)	9 (3%)	0	100	100
2	B	166/183 (91%)	157 (95%)	8 (5%)	1 (1%)	25	47
All	All	478/508 (94%)	460 (96%)	17 (4%)	1 (0%)	47	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	ASP

### 5.3.2 Protein sidechains [i](#)

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	264/272 (97%)	262 (99%)	2 (1%)	81	92
2	B	143/157 (91%)	142 (99%)	1 (1%)	84	94
All	All	407/429 (95%)	404 (99%)	3 (1%)	84	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	123	MET
2	B	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	224	ASN
1	A	291	ASN
2	B	12	ASN
2	B	42	GLN
2	B	60	ASN
2	B	62	GLN
2	B	125	GLN
2	B	142	HIS

### 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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	MOH	A	3002	3	1,1,1	0.17	0	-		
3	SIA	A	3001	4	20,20,21	2.09	4 (20%)	24,28,31	1.76	8 (33%)
5	NAG	A	3004	1	14,14,15	0.78	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	B	201	2	14,14,15	1.53	2 (14%)	17,19,21	1.61	1 (5%)
5	NAG	A	3003	1	14,14,15	0.35	0	17,19,21	0.37	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	A	3001	4	-	1/18/34/38	0/1/1/1
5	NAG	A	3003	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	A	3004	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3001	SIA	C2-C1	7.18	1.58	1.52
5	B	201	NAG	C1-C2	4.95	1.59	1.52
3	A	3001	SIA	O6-C2	3.73	1.48	1.43
3	A	3001	SIA	C7-C6	2.86	1.56	1.53
5	B	201	NAG	O5-C1	2.77	1.48	1.43
5	A	3004	NAG	O5-C1	2.30	1.47	1.43
3	A	3001	SIA	C6-C5	2.18	1.56	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	NAG	C1-O5-C5	6.07	120.41	112.19
3	A	3001	SIA	C6-O6-C2	4.41	120.78	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3004	NAG	C1-O5-C5	3.49	116.93	112.19
3	A	3001	SIA	C3-C4-C5	-2.85	108.02	111.46
3	A	3001	SIA	O6-C2-C3	-2.77	106.65	110.46
3	A	3001	SIA	O1A-C1-C2	-2.68	116.23	122.57
3	A	3001	SIA	O1B-C1-O1A	2.67	130.15	124.09
3	A	3001	SIA	O10-C10-N5	2.02	125.67	121.95
3	A	3001	SIA	O4-C4-C3	2.02	114.94	109.94
3	A	3001	SIA	O10-C10-C11	-2.01	118.33	122.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

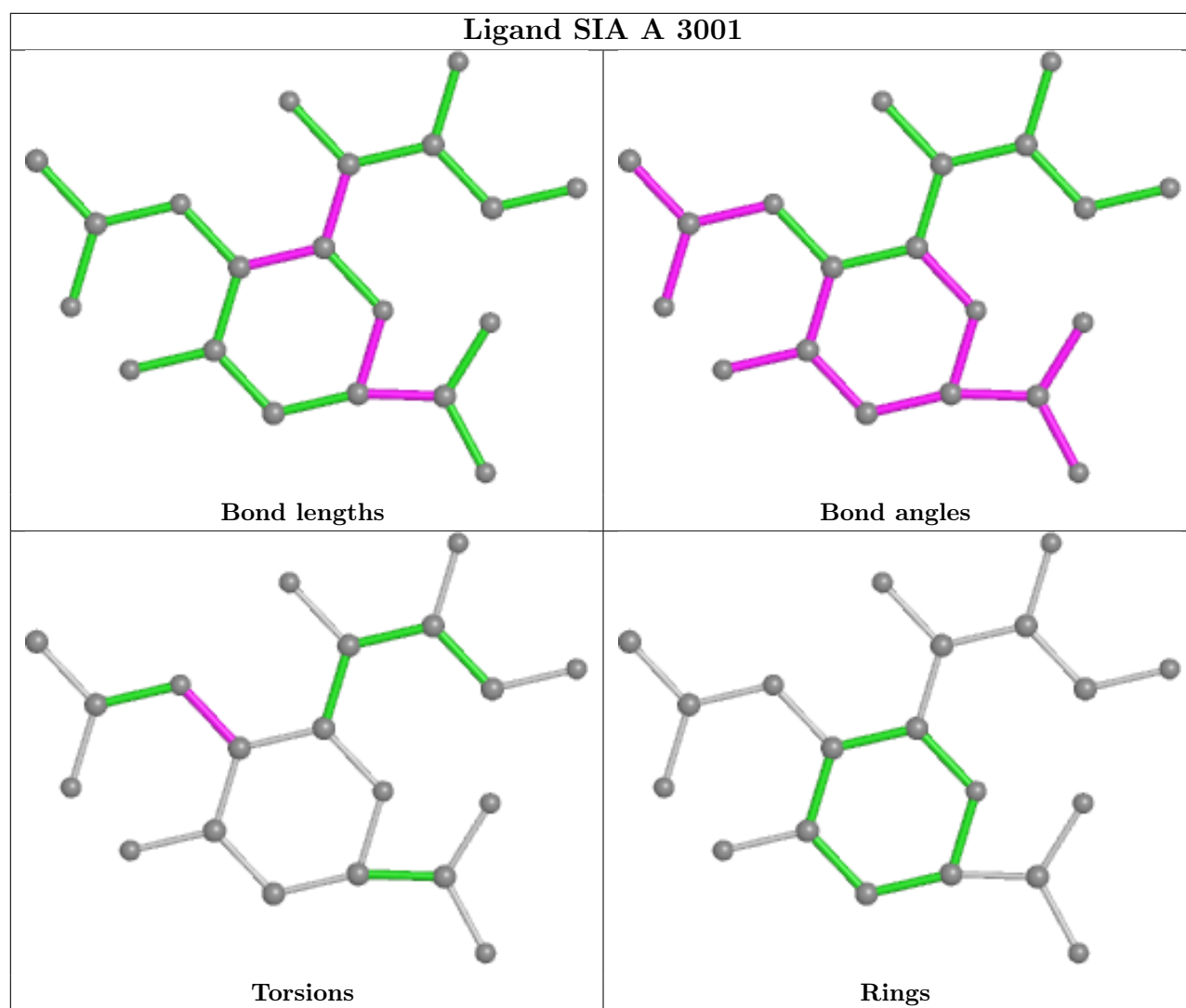
Mol	Chain	Res	Type	Atoms
5	A	3004	NAG	C4-C5-C6-O6
5	A	3004	NAG	O5-C5-C6-O6
3	A	3001	SIA	C6-C5-N5-C10

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	SIA	1	0
5	B	201	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	314/325 (96%)	0.10	6 (1%) 66 62	54, 83, 127, 163	0
2	B	168/183 (91%)	1.09	37 (22%) 0 0	53, 120, 186, 210	0
All	All	482/508 (94%)	0.45	43 (8%) 9 6	53, 88, 165, 210	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	27	GLN	5.1
2	B	168	GLN	5.0
1	A	210	GLN	4.4
1	A	15	LEU	4.4
2	B	161	LYS	4.3
2	B	124	ARG	4.2
2	B	35	ALA	4.1
2	B	120	GLU	4.0
2	B	162	TYR	3.9
2	B	26	HIS	3.8
2	B	60	ASN	3.6
2	B	146	ASP	3.4
2	B	24	PHE	3.4
2	B	139	GLU	3.3
2	B	33	GLY	3.1
2	B	147	ASP	3.0
2	B	25	ARG	3.0
1	A	14	CYS	3.0
2	B	32	GLU	3.0
2	B	23	GLY	2.9
2	B	157	TYR	2.9
2	B	152	ILE	2.8
2	B	166	ALA	2.8
2	B	126	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	148	CYS	2.8
2	B	142	HIS	2.7
2	B	31	GLY	2.6
2	B	132	GLU	2.6
1	A	127	TYR	2.6
2	B	3	PHE	2.6
2	B	136	GLY	2.5
2	B	34	THR	2.5
2	B	116	ASP	2.4
2	B	121	ARG	2.3
2	B	29	ALA	2.3
1	A	199	ASN	2.3
1	A	289	ILE	2.3
2	B	17	LEU	2.3
2	B	118	LEU	2.2
2	B	102	MET	2.2
2	B	30	GLN	2.2
2	B	160	SER	2.1
2	B	163	ARG	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](#)

There are no monosaccharides in this entry.

## 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. 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.

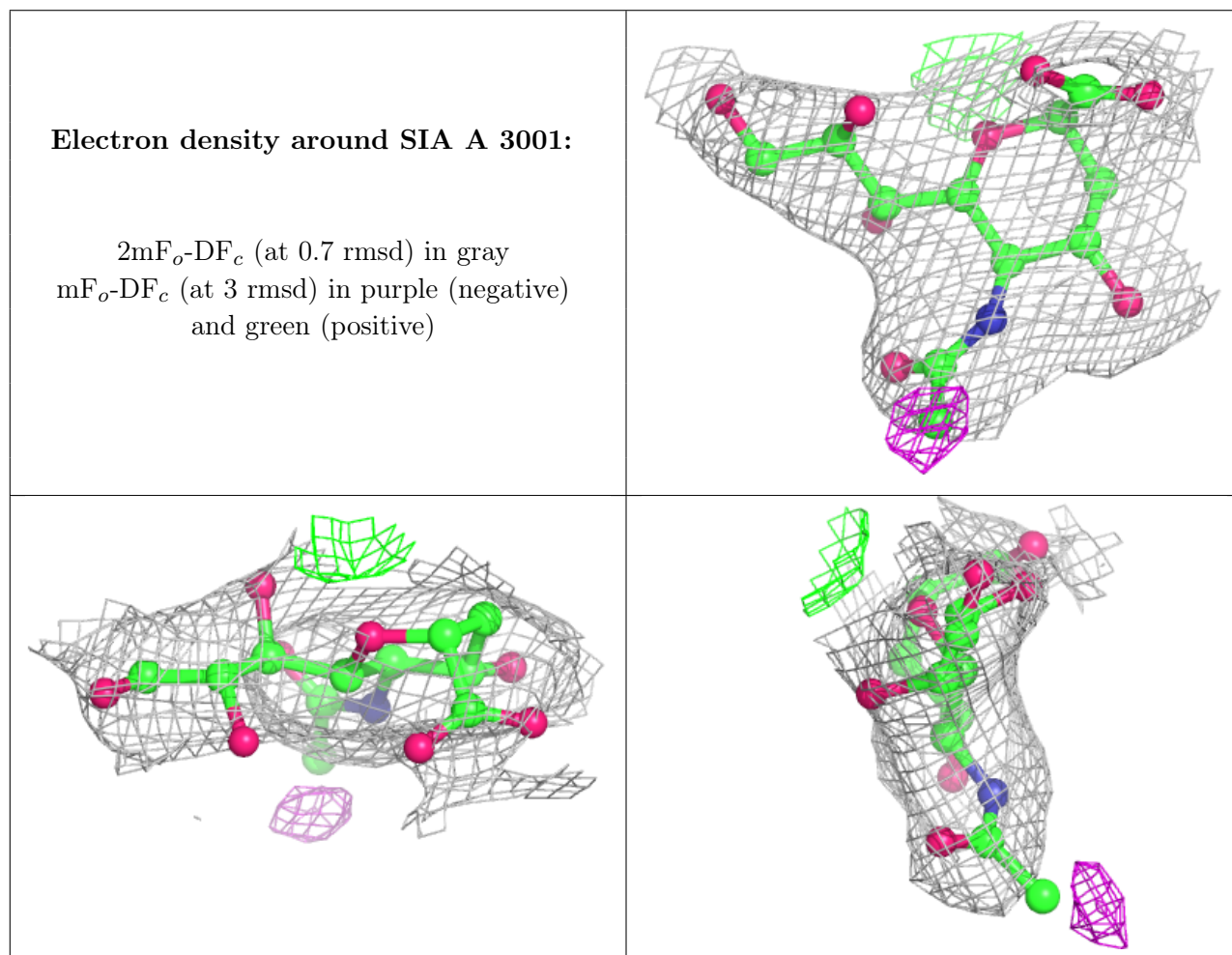
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	B	201	14/15	0.78	0.16	80,97,113,116	0
4	MOH	A	3002	2/2	0.80	0.18	133,133,133,136	0
5	NAG	A	3004	14/15	0.84	0.26	114,130,139,147	0
5	NAG	A	3003	14/15	0.88	0.23	115,128,133,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SIA	A	3001	20/21	0.89	0.23	88,109,148,149	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.