



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:29 AM GMT

PDB ID : 3M5I  
Title : Crystal structure of a H7 influenza virus hemagglutinin complexed with 6SLN  
Authors : Yang, H.; Chen, L.M.; Carney, P.J.; Donis, R.O.; Stevens, J.  
Deposited on : 2010-03-12  
Resolution : 3.00 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

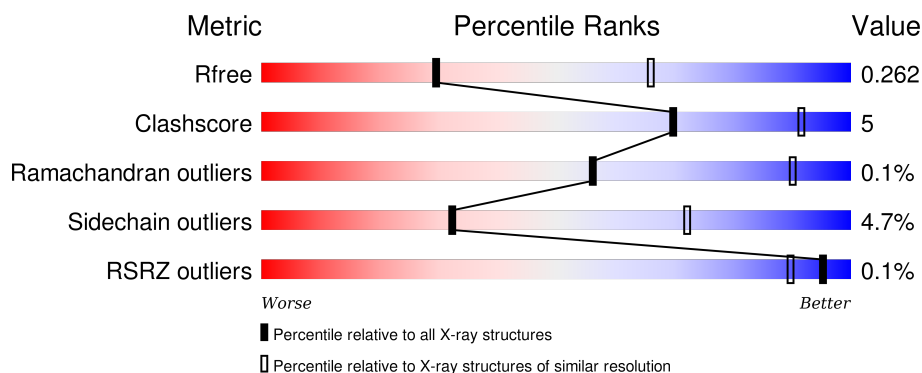
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	317	 80% 16% . .
1	C	317	 80% 16% . .
1	E	317	 81% 15% . .
2	B	182	 85% 12% .
2	D	182	 80% 14% 5%

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Mol	Chain	Length	Quality of chain
2	F	182	 84% 10% 6%

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	SIA	C	1	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11645 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2383	1482	431	457	13			
1	C	309	Total	C	N	O	S	0	0	0
			2383	1482	431	457	13			
1	E	309	Total	C	N	O	S	0	0	0
			2383	1482	431	457	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP B7NY59
A	8	ASP	-	EXPRESSION TAG	UNP B7NY59
A	9	PRO	-	EXPRESSION TAG	UNP B7NY59
A	216	ASN	SER	SEE REMARK 999	UNP B7NY59
A	257	THR	ALA	SEE REMARK 999	UNP B7NY59
A	309	VAL	ILE	SEE REMARK 999	UNP B7NY59
C	7	ALA	-	EXPRESSION TAG	UNP B7NY59
C	8	ASP	-	EXPRESSION TAG	UNP B7NY59
C	9	PRO	-	EXPRESSION TAG	UNP B7NY59
C	216	ASN	SER	SEE REMARK 999	UNP B7NY59
C	257	THR	ALA	SEE REMARK 999	UNP B7NY59
C	309	VAL	ILE	SEE REMARK 999	UNP B7NY59
E	7	ALA	-	EXPRESSION TAG	UNP B7NY59
E	8	ASP	-	EXPRESSION TAG	UNP B7NY59
E	9	PRO	-	EXPRESSION TAG	UNP B7NY59
E	216	ASN	SER	SEE REMARK 999	UNP B7NY59
E	257	THR	ALA	SEE REMARK 999	UNP B7NY59
E	309	VAL	ILE	SEE REMARK 999	UNP B7NY59

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1415	874	247	287	7			
2	D	172	Total	C	N	O	S	0	0	0
			1393	861	244	281	7			
2	F	171	Total	C	N	O	S	0	0	0
			1384	856	242	279	7			

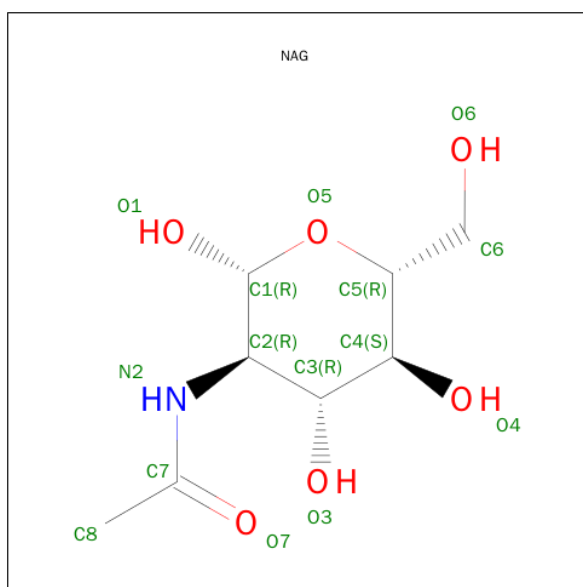
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
B	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
B	179	VAL	-	EXPRESSION TAG	UNP B7NYS1
B	180	PRO	-	EXPRESSION TAG	UNP B7NYS1
B	181	ARG	-	EXPRESSION TAG	UNP B7NYS1
B	182	GLY	-	EXPRESSION TAG	UNP B7NYS1
D	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
D	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
D	179	VAL	-	EXPRESSION TAG	UNP B7NYS1
D	180	PRO	-	EXPRESSION TAG	UNP B7NYS1
D	181	ARG	-	EXPRESSION TAG	UNP B7NYS1
D	182	GLY	-	EXPRESSION TAG	UNP B7NYS1
F	176	GLY	VAL	SEE REMARK 999	UNP B7NYS1
F	177	ARG	LYS	SEE REMARK 999	UNP B7NYS1
F	179	VAL	-	EXPRESSION TAG	UNP B7NYS1
F	180	PRO	-	EXPRESSION TAG	UNP B7NYS1
F	181	ARG	-	EXPRESSION TAG	UNP B7NYS1
F	182	GLY	-	EXPRESSION TAG	UNP B7NYS1

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			32	17	1	14		
3	C	2	Total	C	N	O	0	0
			32	17	1	14		
3	E	2	Total	C	N	O	0	0
			32	17	1	14		

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O	0	0
			13	13		
6	B	10	Total	O	0	0
			10	10		
6	C	7	Total	O	0	0
			7	7		

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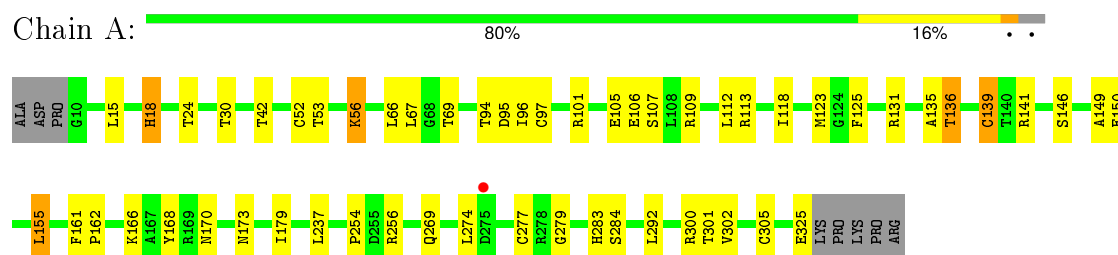
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	9	Total 9	O 9	0	0
6	E	23	Total 23	O 23	0	0
6	F	6	Total 6	O 6	0	0

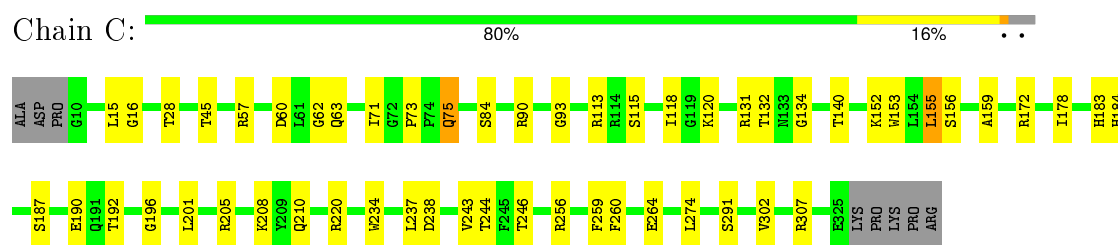
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

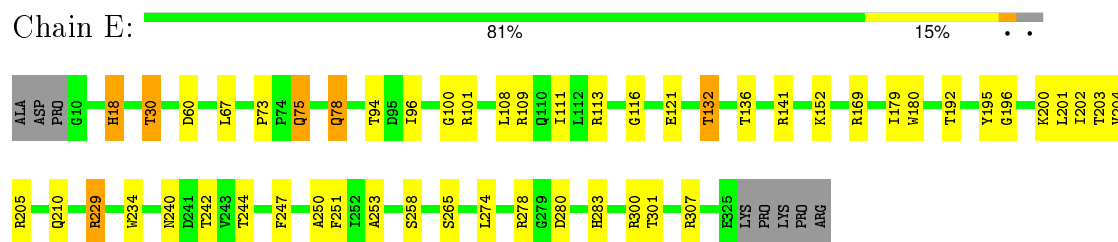
#### • Molecule 1: Hemagglutinin



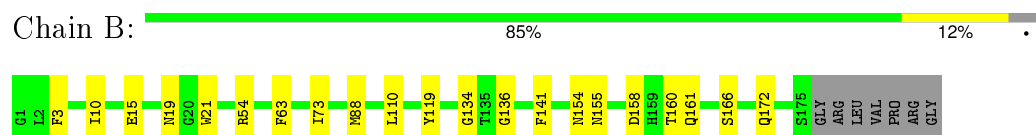
#### • Molecule 1: Hemagglutinin



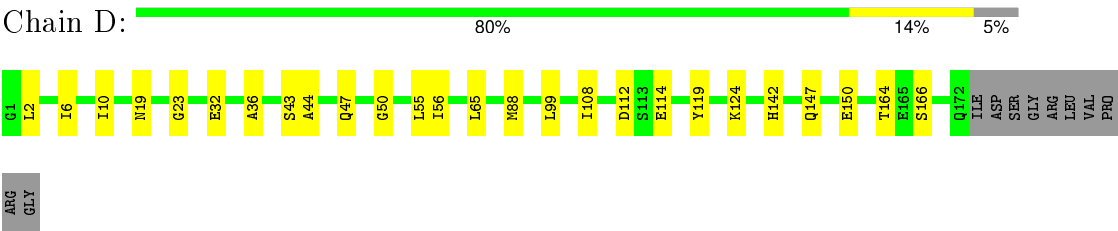
#### • Molecule 1: Hemagglutinin



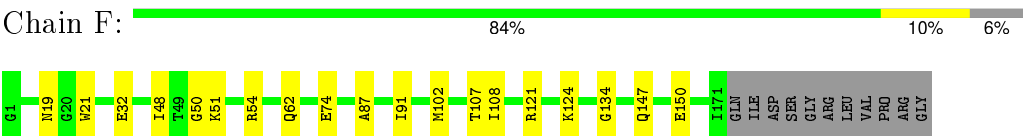
#### • Molecule 2: Hemagglutinin



#### • Molecule 2: Hemagglutinin



● Molecule 2: Hemagglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.60Å 116.53Å 250.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 47.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.0 (50.00-3.00) 88.0 (47.55-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.89 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, $R_{free}$	0.205 , 0.260 0.208 , 0.262	Depositor DCC
$R_{free}$ test set	1779 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 19.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 35200 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.40	0/2431	0.56	0/3286
1	C	0.41	0/2431	0.54	0/3286
1	E	0.41	0/2431	0.57	0/3286
2	B	0.42	0/1439	0.53	0/1940
2	D	0.41	0/1417	0.53	0/1910
2	F	0.41	0/1408	0.55	0/1898
All	All	0.41	0/11557	0.55	0/15606

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	A	2383	0	2340	31	0
1	C	2383	0	2340	30	0
1	E	2383	0	2340	23	0
2	B	1415	0	1321	14	0
2	D	1393	0	1301	18	0
2	F	1384	0	1293	7	0
3	A	32	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	28	0	0
3	E	32	0	28	0	0
4	A	14	0	13	0	0
4	E	14	0	13	0	0
5	B	28	0	25	1	0
5	C	28	0	25	0	0
5	D	28	0	25	0	0
5	F	28	0	25	1	0
6	A	13	0	0	0	0
6	B	10	0	0	0	0
6	C	7	0	0	0	0
6	D	9	0	0	1	0
6	E	23	0	0	0	0
6	F	6	0	0	1	0
All	All	11645	0	11145	103	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 5.

All (103) 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:C:205:ARG:HG2	1:C:210:GLN:HG2	1.51	0.92
1:E:73:PRO:HB2	1:E:75:GLN:OE1	1.80	0.81
1:E:132:THR:HG23	1:E:152:LYS:HD2	1.64	0.79
2:B:158:ASP:OD1	2:B:160:THR:HG22	1.87	0.73
1:A:52:CYS:HB3	1:A:277:CYS:O	1.98	0.64
2:B:88:MET:HE1	2:D:88:MET:HE3	1.80	0.63
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.81	0.62
2:B:172:GLN:HB2	6:F:185:HOH:O	1.99	0.62
1:A:56:LYS:HE2	1:A:279:GLY:O	2.00	0.61
1:C:71:ILE:HG13	1:C:73:PRO:HD3	1.82	0.61
1:C:237:LEU:HD13	1:C:243:VAL:HG23	1.83	0.60
1:E:251:PHE:CE2	1:E:253:ALA:HB2	2.36	0.60
1:A:141:ARG:HH21	1:A:149:ALA:HB2	1.67	0.59
1:A:136:THR:HG23	1:A:139:CYS:HB2	1.83	0.59
2:D:147:GLN:O	2:D:150:GLU:HB3	2.02	0.59
1:A:42:THR:HA	1:A:292:LEU:HD22	1.86	0.58
1:A:131:ARG:HB3	1:A:155:LEU:HD12	1.86	0.58
1:A:105:GLU:O	1:A:109:ARG:HG3	2.04	0.57
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ARG:HG2	1:C:210:GLN:CG	2.30	0.55
1:C:187:SER:H	1:C:190:GLU:HG3	1.72	0.55
1:A:141:ARG:NH2	1:A:149:ALA:HB2	2.21	0.54
2:F:51:LYS:NZ	2:F:107:THR:OG1	2.38	0.53
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.43	0.53
1:A:15:LEU:HD13	2:B:119:TYR:HA	1.88	0.53
1:C:192:THR:HA	1:C:196:GLY:O	2.08	0.53
2:D:23:GLY:HA2	2:D:36:ALA:HA	1.90	0.52
1:A:30:THR:O	2:F:50:GLY:HA3	2.09	0.52
2:B:88:MET:CE	2:D:88:MET:HE3	2.41	0.51
1:E:179:ILE:HD13	1:E:234:TRP:HB3	1.92	0.51
1:C:15:LEU:HD22	2:D:119:TYR:HA	1.94	0.50
1:E:180:TRP:CE2	1:E:204:VAL:HG21	2.47	0.50
1:A:170:ASN:HB2	1:A:237:LEU:HD23	1.94	0.49
1:C:291:SER:HB3	2:D:56:ILE:HG23	1.95	0.49
1:C:60:ASP:HB2	1:C:274:LEU:HD11	1.94	0.49
1:E:283:HIS:HB3	1:E:301:THR:HG22	1.94	0.48
1:E:60:ASP:HB2	1:E:274:LEU:HD11	1.96	0.48
1:C:28:THR:HG21	2:D:108:ILE:HD12	1.95	0.48
1:A:135:ALA:HB1	1:A:146:SER:HB2	1.94	0.48
1:E:205:ARG:HG3	1:E:210:GLN:HG2	1.95	0.48
1:E:202:ILE:HG23	1:E:247:PHE:HB3	1.97	0.47
1:E:116:GLY:HA2	1:E:265:SER:HB3	1.96	0.47
1:A:125:PHE:CE2	1:A:166:LYS:HB3	2.50	0.46
1:A:53:THR:HG21	1:A:274:LEU:HD13	1.98	0.46
2:B:134:GLY:HA2	2:F:124:LYS:HD3	1.98	0.46
1:A:325:GLU:HG3	2:B:15:GLU:HG3	1.98	0.46
1:C:62:GLY:HA2	1:C:90:ARG:HG3	1.98	0.46
1:A:269:GLN:O	1:A:284:SER:HA	2.15	0.46
1:C:57:ARG:O	1:C:84:SER:HB2	2.16	0.45
1:E:192:THR:HA	1:E:196:GLY:O	2.17	0.45
2:D:50:GLY:HA3	1:E:30:THR:O	2.17	0.45
1:E:67:LEU:HD22	1:E:108:LEU:HD23	1.99	0.45
2:D:47:GLN:HA	1:E:30:THR:HG23	1.98	0.44
1:C:302:VAL:HG11	2:D:65:LEU:HG	2.00	0.44
1:C:63:GLN:HG2	1:C:75:GLN:HB3	2.00	0.44
1:A:305:CYS:HB2	2:B:63:PHE:CD2	2.53	0.44
2:D:44:ALA:HB2	2:D:114:GLU:HG3	1.99	0.44
1:E:78:GLN:H	1:E:78:GLN:HG3	1.64	0.44
1:A:67:LEU:HD23	1:A:112:LEU:HD12	1.98	0.44
2:B:158:ASP:O	2:B:161:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:87:ALA:O	2:F:91:ILE:HG13	2.17	0.43
2:D:124:LYS:HD2	2:F:134:GLY:HA2	2.00	0.43
1:C:184:HIS:O	1:C:220:ARG:HA	2.19	0.43
1:C:131:ARG:HB2	1:C:155:LEU:HD12	2.01	0.43
2:D:142:HIS:HB3	2:D:166:SER:HB3	2.01	0.43
1:A:123:MET:HA	1:A:168:TYR:CE1	2.53	0.43
1:A:69:THR:HB	1:A:118:ILE:HD11	2.01	0.43
1:C:307:ARG:H	1:C:307:ARG:HD2	1.84	0.43
1:A:30:THR:HG22	2:F:51:LYS:HG3	2.00	0.43
1:E:195:TYR:CZ	1:E:250:ALA:HA	2.54	0.43
1:E:300:ARG:HH21	5:F:184:NAG:H81	1.83	0.43
1:E:109:ARG:O	1:E:113:ARG:HG3	2.20	0.42
1:E:18:HIS:CD2	2:F:21:TRP:HA	2.55	0.42
1:A:161:PHE:HA	1:A:162:PRO:HD3	1.89	0.42
1:C:156:SER:HB3	1:C:159:ALA:HB3	2.01	0.42
1:C:113:ARG:HD2	6:D:188:HOH:O	2.21	0.41
1:A:300:ARG:NH2	5:B:183:NAG:H5	2.35	0.41
1:C:132:THR:HB	1:C:152:LYS:HE3	2.01	0.41
1:A:66:LEU:HD11	1:A:112:LEU:HB3	2.02	0.41
1:A:179:ILE:O	1:A:254:PRO:HB3	2.20	0.41
1:A:150:GLU:OE1	1:A:256:ARG:HD3	2.20	0.41
2:B:10:ILE:HD13	2:B:136:GLY:HA3	2.00	0.41
1:A:106:GLU:HG2	2:B:73:ILE:HG21	2.02	0.41
1:C:172:ARG:HG3	1:C:259:PHE:CE2	2.55	0.41
2:B:3:PHE:CZ	2:D:2:LEU:HB3	2.56	0.41
1:C:153:TRP:HZ2	1:C:183:HIS:CE1	2.38	0.41
2:B:141:PHE:O	2:B:166:SER:HA	2.20	0.41
1:C:120:LYS:HB2	1:C:256:ARG:HH21	1.86	0.41
2:D:55:LEU:HD22	2:D:99:LEU:HD21	2.03	0.41
1:C:16:GLY:HA2	2:D:10:ILE:HD13	2.03	0.41
1:A:283:HIS:HB3	1:A:301:THR:HG22	2.03	0.41
1:C:178:ILE:O	1:C:234:TRP:HA	2.21	0.41
1:C:115:SER:HB2	1:C:260:PHE:CD1	2.57	0.41
1:E:169:ARG:HH11	1:E:240:ASN:HA	1.85	0.41
2:D:43:SER:O	2:D:47:GLN:HG3	2.21	0.40
1:C:237:LEU:HD22	1:C:243:VAL:HG23	2.04	0.40
1:C:63:GLN:O	1:C:93:GLY:HA2	2.22	0.40
1:A:94:THR:HG22	1:A:96:ILE:H	1.87	0.40
1:E:201:LEU:HD11	1:E:203:THR:HG23	2.03	0.40
1:E:94:THR:HG22	1:E:96:ILE:H	1.86	0.40
1:A:109:ARG:O	1:A:113:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ILE:HD12	1:C:120:LYS:HE3	2.03	0.40
1:E:100:GLY:HA2	1:E:229:ARG:HH11	1.87	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	307/317 (97%)	284 (92%)	23 (8%)	0	100	100
1	C	307/317 (97%)	286 (93%)	21 (7%)	0	100	100
1	E	307/317 (97%)	293 (95%)	14 (5%)	0	100	100
2	B	173/182 (95%)	161 (93%)	12 (7%)	0	100	100
2	D	170/182 (93%)	159 (94%)	11 (6%)	0	100	100
2	F	169/182 (93%)	153 (90%)	15 (9%)	1 (1%)	30	72
All	All	1433/1497 (96%)	1336 (93%)	96 (7%)	1 (0%)	56	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	32	GLU

### 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	264/271 (97%)	252 (96%)	12 (4%)	34	74
1	C	264/271 (97%)	254 (96%)	10 (4%)	40	78
1	E	264/271 (97%)	246 (93%)	18 (7%)	20	56
2	B	150/155 (97%)	145 (97%)	5 (3%)	45	82
2	D	147/155 (95%)	144 (98%)	3 (2%)	63	89
2	F	146/155 (94%)	136 (93%)	10 (7%)	20	56
All	All	1235/1278 (97%)	1177 (95%)	58 (5%)	32	72

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	24	THR
1	A	56	LYS
1	A	95	ASP
1	A	97	CYS
1	A	101	ARG
1	A	107	SER
1	A	136	THR
1	A	139	CYS
1	A	155	LEU
1	A	173	ASN
1	A	302	VAL
2	B	19	ASN
2	B	54	ARG
2	B	110	LEU
2	B	154	ASN
2	B	155	ASN
1	C	45	THR
1	C	75	GLN
1	C	140	THR
1	C	155	LEU
1	C	201	LEU
1	C	208	LYS
1	C	238	ASP
1	C	244	THR
1	C	246	THR
1	C	264	GLU
2	D	19	ASN
2	D	32	GLU
2	D	164	THR

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Mol	Chain	Res	Type
1	E	18	HIS
1	E	30	THR
1	E	75	GLN
1	E	78	GLN
1	E	101	ARG
1	E	111	ILE
1	E	121	GLU
1	E	132	THR
1	E	136	THR
1	E	141	ARG
1	E	200	LYS
1	E	229	ARG
1	E	242	THR
1	E	244	THR
1	E	258	SER
1	E	278	ARG
1	E	280	ASP
1	E	307	ARG
2	F	19	ASN
2	F	48	ILE
2	F	54	ARG
2	F	62	GLN
2	F	74	GLU
2	F	102	MET
2	F	108	ILE
2	F	121	ARG
2	F	147	GLN
2	F	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

14 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	A	1	3	16,20,21	0.38	0	18,28,31	0.92	1 (5%)
3	GAL	A	2	3	12,12,12	0.66	0	17,17,17	1.20	1 (5%)
5	NAG	B	183	2,5	14,14,15	0.43	0	15,19,21	1.69	2 (13%)
5	NAG	B	184	5	14,14,15	0.54	0	15,19,21	1.21	2 (13%)
3	SIA	C	1	3	16,20,21	0.73	0	18,28,31	1.10	2 (11%)
3	GAL	C	2	3	12,12,12	0.53	0	17,17,17	0.86	1 (5%)
5	NAG	C	331	1,5	14,14,15	0.57	0	15,19,21	1.04	2 (13%)
5	NAG	C	332	5	14,14,15	0.60	0	15,19,21	1.50	1 (6%)
5	NAG	D	183	2,5	14,14,15	0.46	0	15,19,21	1.12	1 (6%)
5	NAG	D	184	5	14,14,15	0.45	0	15,19,21	2.08	1 (6%)
3	SIA	E	1	3	16,20,21	0.51	0	18,28,31	0.85	0
3	GAL	E	2	3	12,12,12	0.51	0	17,17,17	0.62	0
5	NAG	F	183	2,5	14,14,15	0.52	0	15,19,21	0.86	1 (6%)
5	NAG	F	184	5	14,14,15	0.59	0	15,19,21	0.96	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
3	SIA	A	1	3	-	0/14/34/38	0/1/1/1
3	GAL	A	2	3	-	0/2/22/22	0/1/1/1
5	NAG	B	183	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	184	5	-	0/6/23/26	0/1/1/1
3	SIA	C	1	3	-	0/14/34/38	0/1/1/1
3	GAL	C	2	3	-	0/2/22/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	183	2,5	-	0/6/23/26	0/1/1/1
5	NAG	D	184	5	-	0/6/23/26	0/1/1/1
3	SIA	E	1	3	-	0/14/34/38	0/1/1/1
3	GAL	E	2	3	-	0/2/22/22	0/1/1/1
5	NAG	F	183	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	184	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	SIA	C7-C6-C5	-2.47	110.58	114.32
5	B	184	NAG	C3-C4-C5	2.04	113.75	110.20
3	C	1	SIA	O6-C2-C3	2.07	113.83	109.86
5	C	331	NAG	C1-O5-C5	2.12	114.94	112.25
3	C	1	SIA	C8-C7-C6	2.15	117.33	113.01
5	B	184	NAG	C2-N2-C7	2.33	126.04	123.04
5	F	184	NAG	C3-C4-C5	2.47	114.51	110.20
5	F	183	NAG	C1-O5-C5	2.49	115.41	112.25
5	C	331	NAG	C4-C3-C2	2.63	115.32	111.23
5	B	183	NAG	C3-C4-C5	2.78	115.05	110.20
3	C	2	GAL	O5-C5-C6	3.01	113.96	106.36
5	D	183	NAG	C1-O5-C5	3.12	116.21	112.25
3	A	2	GAL	C3-C4-C5	3.29	115.93	110.20
5	C	332	NAG	C1-O5-C5	4.69	118.20	112.25
5	B	183	NAG	C1-O5-C5	5.25	118.91	112.25
5	D	184	NAG	C1-O5-C5	7.42	121.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	183	NAG	1	0
5	F	184	NAG	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	A	331	1	14,14,15	0.50	0	15,19,21	1.52	4 (26%)
4	NAG	E	331	1	14,14,15	0.58	0	15,19,21	1.15	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	A	331	1	-	0/6/23/26	0/1/1/1
4	NAG	E	331	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	331	NAG	C4-C3-C2	-2.28	107.68	111.23
4	A	331	NAG	C1-O5-C5	2.11	114.92	112.25
4	A	331	NAG	C3-C2-N2	2.22	115.88	110.56
4	E	331	NAG	C2-N2-C7	2.80	126.64	123.04
4	A	331	NAG	C2-N2-C7	3.44	127.46	123.04

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 ⓘ

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	309/317 (97%)	-0.45	1 (0%) 94 84	19, 37, 51, 57	0
1	C	309/317 (97%)	-0.46	0 100 100	18, 36, 47, 51	0
1	E	309/317 (97%)	-0.55	0 100 100	16, 37, 47, 52	0
2	B	175/182 (96%)	-0.49	0 100 100	25, 44, 62, 67	0
2	D	172/182 (94%)	-0.40	0 100 100	28, 45, 55, 67	0
2	F	171/182 (93%)	-0.36	0 100 100	24, 46, 54, 61	0
All	All	1445/1497 (96%)	-0.46	1 (0%) 95 90	16, 39, 52, 67	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	2.7

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SIA	C	1	20/21	0.84	0.29	2.29	75,87,94,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SIA	E	1	20/21	0.91	0.26	1.81	57,72,86,87	0
3	SIA	A	1	20/21	0.91	0.25	1.44	80,88,96,98	0
5	NAG	F	183	14/15	0.93	0.17	0.19	63,73,81,82	0
5	NAG	B	183	14/15	0.90	0.16	-0.21	56,68,78,89	0
5	NAG	D	183	14/15	0.89	0.18	-0.82	73,82,87,88	0
5	NAG	F	184	14/15	0.86	0.24	-	74,89,93,94	0
5	NAG	B	184	14/15	0.74	0.48	-	98,104,107,109	0
3	GAL	C	2	12/12	0.64	0.29	-	110,113,115,116	0
3	GAL	A	2	12/12	0.74	0.26	-	97,100,102,103	0
5	NAG	C	331	14/15	0.90	0.20	-	77,87,90,92	0
3	GAL	E	2	12/12	0.66	0.30	-	106,115,117,117	0
5	NAG	C	332	14/15	0.71	0.28	-	86,93,96,96	0
5	NAG	D	184	14/15	0.80	0.23	-	84,95,100,101	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( $\text{\AA}^2$ )	Q<0.9
4	NAG	E	331	14/15	0.91	0.15	-	76,86,88,89	0
4	NAG	A	331	14/15	0.83	0.27	-	76,84,89,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.