



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:17 PM GMT

PDB ID : 5A3I  
Title : Crystal Structure of a Complex formed between FLD194 Fab and Transmissible Mutant H5 Haemagglutinin  
Authors : Xiong, X.; Corti, D.; Liu, J.; Pinna, D.; Foglierini, M.; Calder, L.J.; Martin, S.R.; Lin, Y.P.; Walker, P.A.; Collins, P.J.; Monne, I.; Suguitan Jr, A.L.; Santos, C.; Temperton, N.J.; Subbarao, K.; Lanzavecchia, A.; Gamblin, S.J.; Skehel, J.J.  
Deposited on : 2015-06-01  
Resolution : 2.89 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

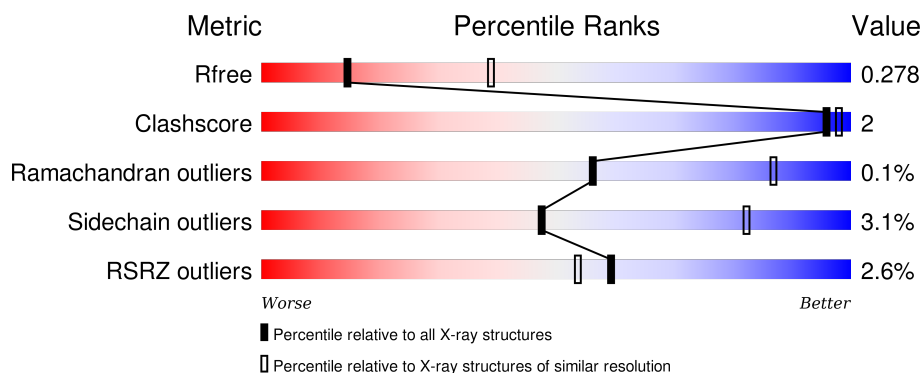
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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	328	<div> <div>3%</div> <div>94%</div> <div>6%</div> <div>• • •</div> </div>
1	E	328	<div> <div>3%</div> <div>91%</div> <div>6%</div> <div>• •</div> </div>
2	B	166	<div> <div>7%</div> <div>94%</div> <div>5%</div> <div>•</div> </div>
3	C	230	<div> <div>%</div> <div>95%</div> <div>• •</div> </div>
3	G	230	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	219	<div><div></div><div>93%</div><div>7%</div></div>
4	H	219	<div>%<div><div></div><div>95%</div><div>5%</div></div></div>
5	F	166	<div>5%<div><div></div><div>93%</div><div>6%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14561 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	323	Total	C	N	O	S	0	0	0
			2555	1617	437	486	15			
1	E	323	Total	C	N	O	S	0	0	0
			2563	1623	439	486	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	EXPRESSION TAG	UNP A5A5M5
A	0	PRO	-	EXPRESSION TAG	UNP A5A5M5
A	325	THR	-	EXPRESSION TAG	UNP A5A5M5
A	326	ARG	-	EXPRESSION TAG	UNP A5A5M5
A	154	ASP	ASN	CONFLICT	UNP A5A5M5
A	220	LYS	ASN	CONFLICT	UNP A5A5M5
A	222	LEU	GLN	CONFLICT	UNP A5A5M5
A	315	ILE	THR	CONFLICT	UNP A5A5M5
E	-1	ASP	-	EXPRESSION TAG	UNP A5A5M5
E	0	PRO	-	EXPRESSION TAG	UNP A5A5M5
E	325	THR	-	EXPRESSION TAG	UNP A5A5M5
E	326	ARG	-	EXPRESSION TAG	UNP A5A5M5
E	154	ASP	ASN	CONFLICT	UNP A5A5M5
E	220	LYS	ASN	CONFLICT	UNP A5A5M5
E	222	LEU	GLN	CONFLICT	UNP A5A5M5
E	315	ILE	THR	CONFLICT	UNP A5A5M5

- Molecule 2 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1331	830	227	266	8			

- Molecule 3 is a protein called ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1695	1075	280	332	8			
3	G	226	Total	C	N	O	S	0	0	0
			1695	1075	280	332	8			

- Molecule 4 is a protein called ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	218	Total	C	N	O	S	0	0	0
			1667	1044	282	335	6			
4	H	218	Total	C	N	O	S	0	0	0
			1663	1041	281	335	6			

- Molecule 5 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	166	Total	C	N	O	S	0	0	0
			1322	822	228	264	8			

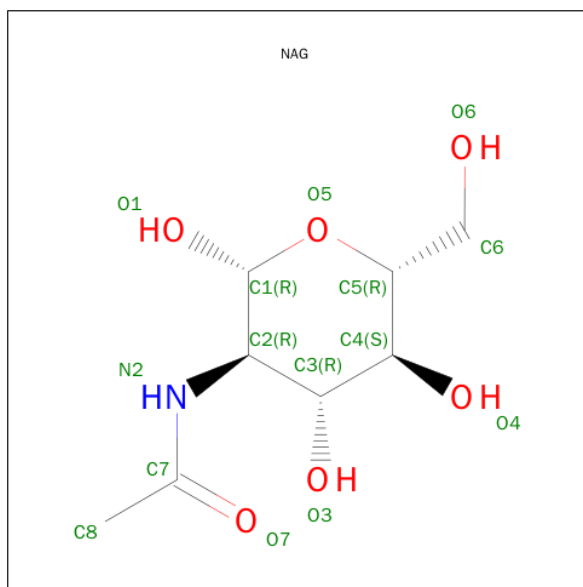
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	68	LYS	ARG	CONFLICT	UNP A5A5M5

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

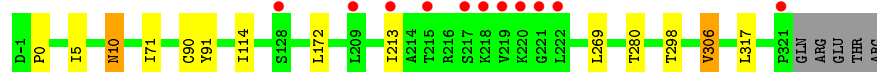


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

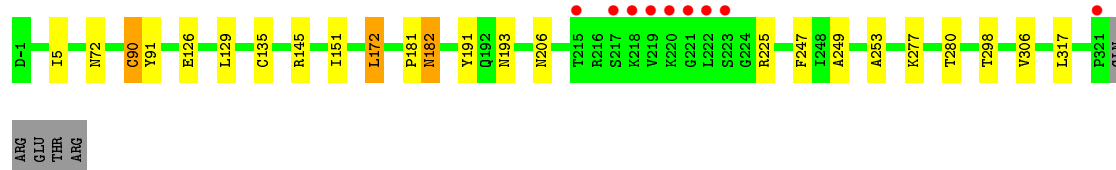
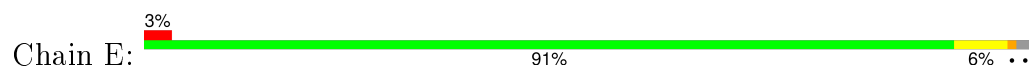
### 3 Residue-property plots [i](#)

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

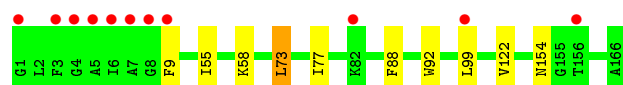
- Molecule 1: HEMAGGLUTININ



- Molecule 1: HEMAGGLUTININ



- Molecule 2: HEMAGGLUTININ



- Molecule 3: ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN



- Molecule 3: ANTI-HAEMAGGLUTININ HA1 FAB HEAVY CHAIN



- Molecule 4: ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN

Chain D: 

93%

7%



• Molecule 4: ANTI-HAEMAGGLUTININ HA1 FAB LIGHT CHAIN

Chain H: 

%

95%

5%



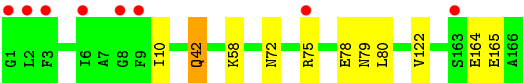
• Molecule 5: HEMAGGLUTININ

Chain F: 

5%

93%

6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.75Å 87.70Å 100.90Å 78.67° 84.66° 73.91°	Depositor
Resolution (Å)	83.33 – 2.89 83.28 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.4 (83.33-2.89) 86.6 (83.28-2.89)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.244 , 0.277 0.246 , 0.278	Depositor DCC
$R_{free}$ test set	2901 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 16.0	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	0 of 57328 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	14561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 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	0.26	0/2618	0.43	0/3560
1	E	0.26	0/2626	0.44	0/3568
2	B	0.28	0/1358	0.42	0/1829
3	C	0.25	0/1741	0.44	0/2374
3	G	0.26	0/1741	0.46	0/2374
4	D	0.26	0/1703	0.47	0/2312
4	H	0.26	0/1699	0.44	0/2308
5	F	0.28	0/1348	0.43	0/1815
All	All	0.26	0/14834	0.44	0/20140

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	2555	0	2491	7	0
1	E	2563	0	2514	8	0
2	B	1331	0	1226	5	0
3	C	1695	0	1653	3	0
3	G	1695	0	1653	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1667	0	1629	2	0
4	H	1663	0	1618	3	0
5	F	1322	0	1217	6	0
6	A	56	0	50	1	0
7	E	14	0	13	0	0
All	All	14561	0	14064	43	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 2.

All (43) 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)
3:G:137:ALA:HB1	3:G:138:PRO:CD	2.20	0.70
1:E:90:CYS:SG	1:E:91:TYR:N	2.65	0.70
1:A:306:VAL:HG13	2:B:92:TRP:CZ3	2.28	0.69
1:E:5:ILE:HD11	5:F:122:VAL:HG21	1.81	0.62
5:F:42:GLN:HA	5:F:42:GLN:HE21	1.61	0.62
3:G:137:ALA:HB1	3:G:138:PRO:HD2	1.82	0.61
2:B:73:LEU:CD2	2:B:77:ILE:HD13	2.33	0.59
6:A:1165:NAG:H61	6:A:1166:NAG:H2	1.86	0.58
4:H:38:LEU:HD22	4:H:76:PHE:CG	2.43	0.54
3:G:139:SER:HA	3:G:140:SER:CB	2.39	0.52
4:H:54:TYR:O	4:H:58:ASN:HB2	2.10	0.52
3:C:32:TYR:CD2	3:C:101:SER:HB2	2.45	0.52
5:F:79:ASN:N	5:F:80:LEU:HB3	2.26	0.50
3:G:137:ALA:CB	3:G:138:PRO:CD	2.90	0.49
3:G:138:PRO:HG3	3:G:150:LEU:HB3	1.96	0.48
1:E:280:THR:HG22	1:E:298:THR:HG22	1.95	0.48
5:F:164:GLU:N	5:F:165:GLU:HA	2.30	0.46
3:C:35:GLY:HA3	3:C:50:ILE:HG22	1.97	0.46
5:F:78:GLU:C	5:F:80:LEU:HB3	2.37	0.46
1:A:280:THR:HG22	1:A:298:THR:HG22	1.98	0.45
3:G:204:GLN:HA	3:G:204:GLN:HE21	1.79	0.45
1:E:172:LEU:HD12	1:E:253:ALA:HB1	1.97	0.45
4:D:54:TYR:O	4:D:58:ASN:HB2	2.16	0.44
1:A:114:ILE:HD11	1:A:172:LEU:HD11	1.99	0.44
1:E:247:PHE:CE2	1:E:249:ALA:HB2	2.52	0.44
3:G:10:GLU:HG3	3:G:18:LEU:HD11	1.99	0.43
2:B:55:ILE:HD11	2:B:99:LEU:HG	2.00	0.43
4:D:38:LEU:HD22	4:D:76:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD11	2:B:122:VAL:HG21	2.00	0.43
1:A:10:ASN:N	1:A:10:ASN:HD22	2.16	0.42
2:B:73:LEU:HD12	2:B:88:PHE:CZ	2.55	0.42
3:G:213:LYS:N	3:G:214:PRO:HD2	2.35	0.41
1:E:182:ASN:N	1:E:182:ASN:OD1	2.54	0.41
1:E:193:ASN:N	1:E:193:ASN:HD22	2.19	0.41
1:A:213:ILE:HD12	1:A:213:ILE:N	2.36	0.41
5:F:42:GLN:HE21	5:F:42:GLN:CA	2.27	0.41
3:G:139:SER:HA	3:G:140:SER:HB3	2.01	0.41
3:G:141:LYS:HA	3:G:142:SER:HA	1.88	0.40
3:G:35:GLY:HA3	3:G:50:ILE:HG22	2.01	0.40
3:C:190:LEU:HD12	3:C:190:LEU:C	2.42	0.40
1:E:126:GLU:HG2	1:E:129:LEU:HD22	2.02	0.40
1:A:90:CYS:SG	1:A:91:TYR:N	2.95	0.40
4:H:29:LEU:HA	4:H:97:LEU:HD22	2.02	0.40

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	321/328 (98%)	308 (96%)	13 (4%)	0	100	100
1	E	321/328 (98%)	305 (95%)	16 (5%)	0	100	100
2	B	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
3	C	224/230 (97%)	213 (95%)	11 (5%)	0	100	100
3	G	224/230 (97%)	209 (93%)	14 (6%)	1 (0%)	39	74
4	D	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
4	H	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
5	F	164/166 (99%)	156 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1850/1886 (98%)	1763 (95%)	86 (5%)	1 (0%)	56 87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	137	ALA

### 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	289/296 (98%)	283 (98%)	6 (2%)	61 88
1	E	291/296 (98%)	277 (95%)	14 (5%)	31 67
2	B	139/141 (99%)	135 (97%)	4 (3%)	50 83
3	C	191/196 (97%)	188 (98%)	3 (2%)	70 91
3	G	191/196 (97%)	188 (98%)	3 (2%)	70 91
4	D	190/191 (100%)	179 (94%)	11 (6%)	25 58
4	H	189/191 (99%)	185 (98%)	4 (2%)	61 88
5	F	137/141 (97%)	132 (96%)	5 (4%)	42 78
All	All	1617/1648 (98%)	1567 (97%)	50 (3%)	47 82

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	PRO
1	A	10	ASN
1	A	71	ILE
1	A	269	LEU
1	A	306	VAL
1	A	317	LEU
2	B	9	PHE
2	B	58	LYS
2	B	73	LEU

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Mol	Chain	Res	Type
2	B	154	ASN
3	C	102	CYS
3	C	117	GLN
3	C	139	SER
4	D	3	VAL
4	D	42	LEU
4	D	55	LEU
4	D	66	ARG
4	D	77	THR
4	D	94	MET
4	D	109	VAL
4	D	131	LYS
4	D	140	LEU
4	D	159	LEU
4	D	174	LYS
1	E	72	ASN
1	E	90	CYS
1	E	135	CYS
1	E	145	ARG
1	E	151	ILE
1	E	172	LEU
1	E	181	PRO
1	E	182	ASN
1	E	191	TYR
1	E	206	ASN
1	E	225	ARG
1	E	277	LYS
1	E	306	VAL
1	E	317	LEU
5	F	10	ILE
5	F	42	GLN
5	F	58	LYS
5	F	72	ASN
5	F	75	ARG
3	G	117	GLN
3	G	201	LEU
3	G	204	GLN
4	H	131	LYS
4	H	140	LEU
4	H	152	GLN
4	H	159	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	10	ASN
1	A	146	ASN
1	A	236	ASN
2	B	60	ASN
2	B	62	GLN
2	B	154	ASN
3	C	176	HIS
4	D	142	ASN
4	D	203	HIS
1	E	84	ASN
1	E	168	ASN
1	E	206	ASN
5	F	42	GLN
5	F	60	ASN
5	F	72	ASN
3	G	204	GLN
4	H	47	GLN
4	H	152	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 ⓘ

4 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
6	NAG	A	1023	1,6	14,14,15	0.46	0	15,19,21	0.72	0
6	NAG	A	1024	6	14,14,15	0.48	0	15,19,21	0.67	0
6	NAG	A	1165	1,6	14,14,15	0.59	0	15,19,21	1.85	5 (33%)
6	NAG	A	1166	6	14,14,15	0.63	0	15,19,21	0.81	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
6	NAG	A	1023	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1024	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1165	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1166	6	-	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(°)
6	A	1165	NAG	O4-C4-C3	-3.78	101.84	110.36
6	A	1165	NAG	C8-C7-N2	2.14	120.20	116.10
6	A	1165	NAG	C4-C3-C2	2.33	114.95	111.34
6	A	1165	NAG	O4-C4-C5	2.43	115.62	109.23
6	A	1165	NAG	C1-O5-C5	3.05	116.62	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1165	NAG	1	0
6	A	1166	NAG	1	0

## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
7	NAG	E	1168	1	14,14,15	0.47	0	15,19,21	1.06	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
7	NAG	E	1168	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	E	1168	NAG	C1-O5-C5	2.25	115.45	112.14

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	A	323/328 (98%)	0.14	11 (3%) 49 41	35, 54, 108, 178	0
1	E	323/328 (98%)	0.18	9 (2%) 56 50	31, 61, 84, 127	0
2	B	166/166 (100%)	0.36	11 (6%) 22 16	38, 81, 125, 159	0
3	C	226/230 (98%)	-0.06	3 (1%) 79 78	33, 44, 67, 90	0
3	G	226/230 (98%)	0.09	4 (1%) 71 68	47, 64, 102, 126	0
4	D	218/219 (99%)	-0.09	0 100 100	29, 47, 59, 84	0
4	H	218/219 (99%)	0.04	2 (0%) 85 84	47, 68, 92, 111	0
5	F	166/166 (100%)	0.25	8 (4%) 34 28	30, 49, 102, 150	0
All	All	1866/1886 (98%)	0.11	48 (2%) 59 54	29, 57, 102, 178	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	GLY	9.4
3	G	143	THR	6.0
1	E	219	VAL	5.6
1	A	222	LEU	5.3
1	E	215	THR	5.3
3	G	144	SER	5.2
3	C	143	THR	5.0
1	A	220	LYS	5.0
5	F	9	PHE	5.0
3	C	142	SER	5.0
3	G	142	SER	4.5
2	B	6	ILE	4.4
1	A	221	GLY	4.3
5	F	8	GLY	4.2
5	F	3	PHE	4.1
5	F	1	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	219	VAL	3.8
1	E	222	LEU	3.8
1	E	217	SER	3.8
5	F	6	ILE	3.8
2	B	3	PHE	3.7
1	E	218	LYS	3.5
4	H	217	GLY	3.5
2	B	7	ALA	3.2
1	A	215	THR	3.1
2	B	1	GLY	3.0
2	B	156	THR	2.8
1	A	209	LEU	2.8
3	G	148	ALA	2.8
2	B	82	LYS	2.8
2	B	8	GLY	2.8
1	E	321	PRO	2.7
2	B	9	PHE	2.7
1	E	220	LYS	2.7
5	F	2	LEU	2.6
1	A	217	SER	2.6
1	A	218	LYS	2.5
3	C	144	SER	2.4
2	B	5	ALA	2.4
5	F	163	SER	2.3
5	F	75	ARG	2.3
2	B	4	GLY	2.2
1	A	321	PRO	2.2
1	A	128	SER	2.2
4	H	35	TYR	2.1
1	E	223	SER	2.1
2	B	99	LEU	2.0
1	A	213	ILE	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
6	NAG	A	1024	14/15	0.86	0.29	-	51,52,55,56	0
6	NAG	A	1165	14/15	0.93	0.18	-	42,45,48,52	0
6	NAG	A	1023	14/15	0.90	0.18	-	40,45,46,48	0
6	NAG	A	1166	14/15	0.86	0.26	-	56,58,59,60	0

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	E	1168	14/15	0.94	0.23	-	31,33,34,34	0

## 6.5 Other polymers

There are no such residues in this entry.