



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3B2V  
Title : Crystal structure of the extracellular region of the epidermal growth factor receptor in complex with the Fab fragment of IMC-11F8  
Authors : Ferguson, K.M.; Li, S.; Kussie, P.  
Deposited on : 2007-10-19  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

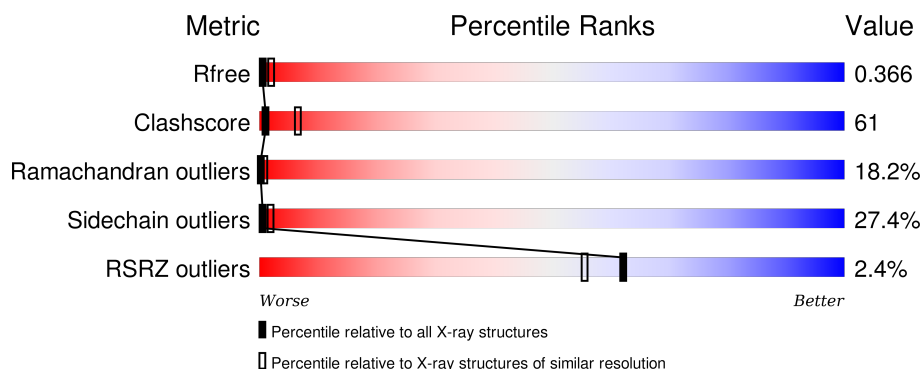
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	L	213	<div> <div>32%</div> <div>44%</div> <div>18%</div> <div>6%</div> </div>
2	H	223	<div> <div>32%</div> <div>40%</div> <div>20%</div> <div>5%</div> </div>
3	A	624	<div> <div>2%</div> <div>17%</div> <div>27%</div> <div>12%</div> <div>40%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NDG	A	3371	X	-	-	-
6	NAG	A	5041	X	-	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5645 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 IMC-11F8 FAB Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1432	883	240	304	5			

- Molecule 2 is a protein called IMC-11F8 FAB Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1533	962	253	313	5			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	375	Total	C	N	O	S	0	0	0
			2559	1561	451	513	34			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	619	HIS	-	EXPRESSION TAG	UNP P00533
A	620	HIS	-	EXPRESSION TAG	UNP P00533
A	621	HIS	-	EXPRESSION TAG	UNP P00533
A	622	HIS	-	EXPRESSION TAG	UNP P00533
A	623	HIS	-	EXPRESSION TAG	UNP P00533
A	624	HIS	-	EXPRESSION TAG	UNP P00533

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			12	8	1	3		

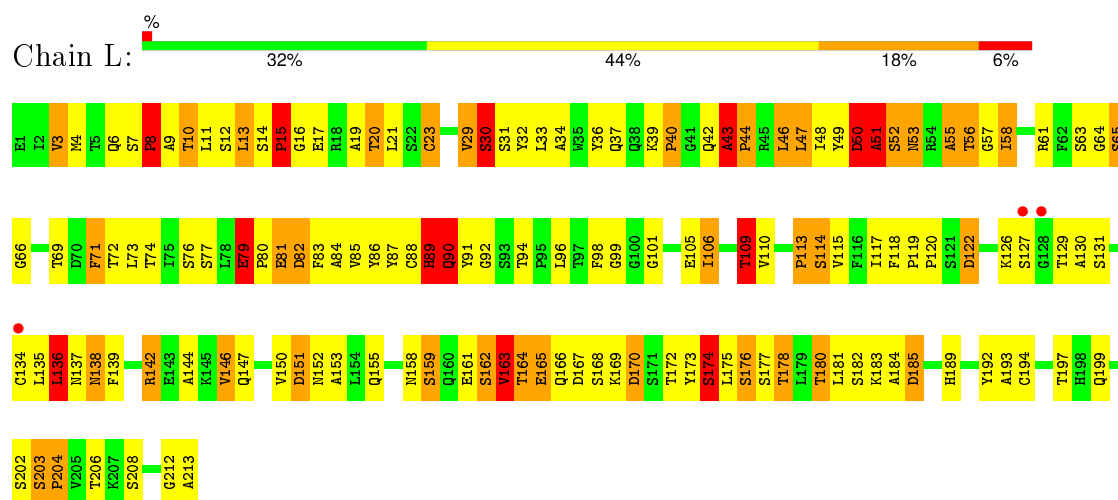
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

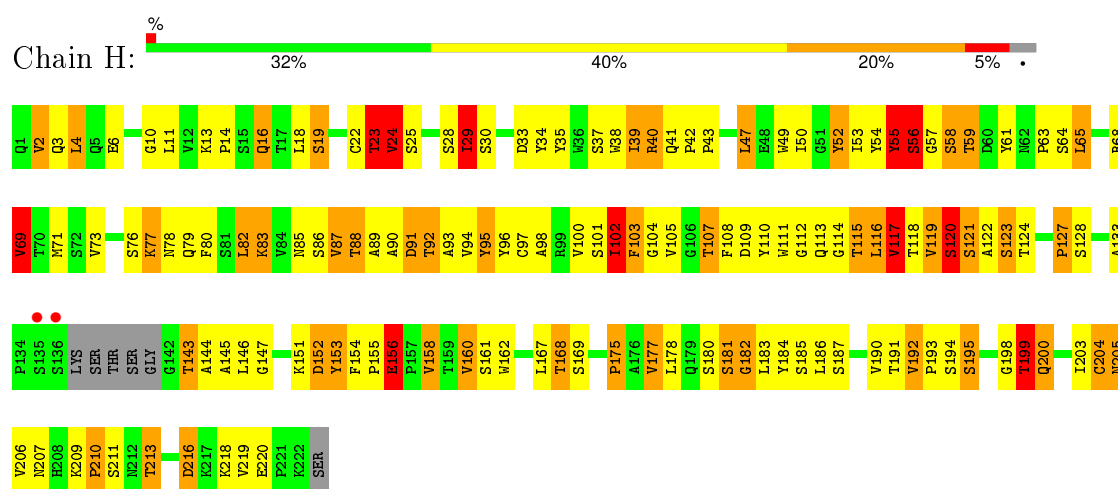
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

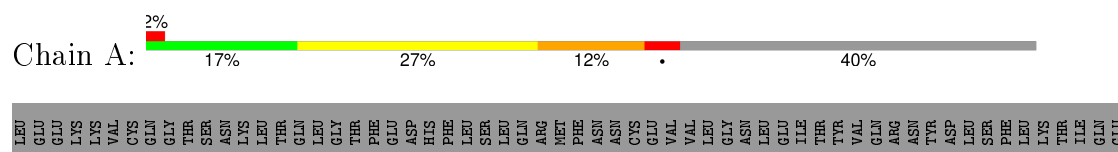
#### • Molecule 1: IMC-11F8 FAB Light chain



#### • Molecule 2: IMC-11F8 FAB Heavy chain



#### • Molecule 3: Epidermal growth factor receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.74Å 266.24Å 156.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.04 – 3.30 41.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.04-3.30) 99.3 (41.04-3.30)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.282 , 0.367 0.285 , 0.366	Depositor DCC
$R_{free}$ test set	1120 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.18 , 70.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21867 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	5645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG

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	L	1.02	1/1460 (0.1%)	1.19	11/2005 (0.5%)
2	H	1.01	2/1570 (0.1%)	1.16	6/2159 (0.3%)
3	A	1.03	2/2607 (0.1%)	1.17	14/3571 (0.4%)
All	All	1.02	5/5637 (0.1%)	1.17	31/7735 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	8
2	H	0	5
3	A	0	11
5	A	1	0
All	All	1	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	534	CYS	CB-SG	-8.21	1.68	1.82
1	L	13	LEU	C-O	5.82	1.34	1.23
2	H	156	GLU	CB-CG	5.45	1.62	1.52
2	H	52	TYR	CE1-CZ	5.18	1.45	1.38
3	A	412	PHE	N-CA	5.11	1.56	1.46

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	382	LEU	CA-CB-CG	-8.96	94.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	82	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	L	138	ASN	N-CA-C	-7.42	90.97	111.00
2	H	24	VAL	CB-CA-C	-7.38	97.38	111.40
3	A	371	LEU	CA-CB-CG	-7.04	99.11	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3371	NDG	C1

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	23	CYS	Peptide
1	L	42	GLN	Peptide
1	L	43	ALA	Peptide
1	L	55	ALA	Peptide
1	L	56	THR	Peptide

## 5.2 Too-close contacts

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	L	1432	0	1229	149	0
2	H	1533	0	1416	198	0
3	A	2559	0	2201	309	0
4	A	39	0	34	0	0
5	A	28	0	25	1	0
6	A	26	0	23	2	0
7	A	28	0	25	1	0
All	All	5645	0	4953	642	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 61.

The worst 5 of 642 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:A:483:HIS:CD2	3:A:496:PRO:HG3	1.52	1.43
1:L:51:ALA:CB	1:L:52:SER:HB2	1.50	1.39
1:L:51:ALA:HB3	1:L:52:SER:CB	1.51	1.38
2:H:24:VAL:HG21	2:H:78:ASN:O	1.24	1.32
2:H:24:VAL:CG2	2:H:78:ASN:O	1.79	1.30

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	L	211/213 (99%)	143 (68%)	33 (16%)	35 (17%)	0	1
2	H	213/223 (96%)	162 (76%)	23 (11%)	28 (13%)	0	2
3	A	373/624 (60%)	207 (56%)	84 (22%)	82 (22%)	0	0
All	All	797/1060 (75%)	512 (64%)	140 (18%)	145 (18%)	0	1

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	9	ALA
1	L	15	PRO
1	L	16	GLY
1	L	32	TYR
1	L	52	SER

### 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	L	135/181 (75%)	94 (70%)	41 (30%)	0	1
2	H	165/192 (86%)	121 (73%)	44 (27%)	0	2
3	A	254/545 (47%)	187 (74%)	67 (26%)	0	2
All	All	554/918 (60%)	402 (73%)	152 (27%)	0	2

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	128	SER
3	A	246	TYR
3	A	525	PHE
2	H	146	LEU
2	H	177	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	334	HIS
3	A	469	ASN
3	A	516	ASN
3	A	314	ASN
3	A	483	HIS

### 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 ⓘ

7 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
4	NAG	A	3281	3,4	14,14,15	1.24	2 (14%)	15,19,21	2.70	7 (46%)
4	NAG	A	3282	4	14,14,15	0.86	0	15,19,21	2.75	4 (26%)
4	BMA	A	3283	4	11,11,12	1.30	1 (9%)	14,15,17	2.25	4 (28%)
5	NDG	A	3371	3,5	14,14,15	0.85	0	15,19,21	2.13	4 (26%)
5	NAG	A	3372	5	14,14,15	0.96	0	15,19,21	2.44	2 (13%)
7	NAG	A	4201	3,7	14,14,15	0.72	0	15,19,21	2.66	9 (60%)
7	NAG	A	4202	7	14,14,15	0.99	0	15,19,21	2.55	6 (40%)

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	3281	3,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3282	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3283	4	-	0/2/19/22	0/1/1/1
5	NDG	A	3371	3,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	3372	5	-	0/6/23/26	0/1/1/1
7	NAG	A	4201	3,7	-	0/6/23/26	0/1/1/1
7	NAG	A	4202	7	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3281	NAG	O5-C1	-2.76	1.39	1.43
4	A	3281	NAG	C2-N2	-2.68	1.41	1.46
4	A	3283	BMA	C2-C3	2.94	1.56	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3372	NAG	C1-O5-C5	-7.12	103.21	112.25
4	A	3282	NAG	C1-O5-C5	-6.85	103.55	112.25
4	A	3281	NAG	C2-N2-C7	-6.51	114.67	123.04
5	A	3371	NDG	O4-C4-C3	-5.90	97.06	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	4202	NAG	C3-C4-C5	-5.27	101.01	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	3371	NDG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3372	NAG	1	0
7	A	4201	NAG	1	0
7	A	4202	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	$\# Z  > 2$
6	NAG	A	3891	3	14,14,15	0.77	0	15,19,21	2.15	4 (26%)
6	NAG	A	5041	3	12,12,15	1.07	0	11,16,21	2.21	5 (45%)

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	3891	3	-	0/6/23/26	0/1/1/1
6	NAG	A	5041	3	1/1/4/7	0/3/20/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	A	3891	NAG	C4-C3-C2	-3.53	105.75	111.23
6	A	5041	NAG	O5-C5-C4	-2.41	105.36	109.53
6	A	5041	NAG	C1-O5-C5	-2.40	108.67	112.38
6	A	5041	NAG	C4-C3-C2	2.45	115.04	111.23
6	A	3891	NAG	C3-C4-C5	2.56	114.66	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	5041	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3891	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	L	213/213 (100%)	-0.22	3 (1%) 78 73	22, 66, 125, 127	0
2	H	217/223 (97%)	-0.36	2 (0%) 85 82	21, 48, 103, 117	0
3	A	375/624 (60%)	-0.21	14 (3%) 45 38	15, 53, 158, 174	0
All	All	805/1060 (75%)	-0.25	19 (2%) 62 55	15, 53, 146, 174	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	596	CYS	4.8
3	A	587	ALA	4.8
3	A	603	GLY	4.3
2	H	136	SER	3.8
3	A	561	TYR	3.6

### 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
4	NAG	A	3281	14/15	0.95	0.22	0.28	31,35,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	A	3283	11/12	0.83	0.15	-	70,75,76,77	0
5	NDG	A	3371	14/15	0.91	0.14	-	78,84,87,88	0
5	NAG	A	3372	14/15	0.81	0.36	-	91,93,94,96	0
7	NAG	A	4201	14/15	0.94	0.14	-	46,50,51,53	0
7	NAG	A	4202	14/15	0.88	0.16	-	58,61,62,62	0
4	NAG	A	3282	14/15	0.83	0.20	-	45,49,57,65	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
6	NAG	A	3891	14/15	0.89	0.16	-	62,68,71,73	0
6	NAG	A	5041	12/15	0.92	0.16	-	39,42,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.