



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:40 AM GMT

PDB ID : 3C09  
Title : Crystal structure the Fab fragment of matuzumab (Fab72000) in complex with domain III of the extracellular region of EGFR  
Authors : Ferguson, K.M.; Schmiedel, J.; Knoechel, T.  
Deposited on : 2008-01-18  
Resolution : 3.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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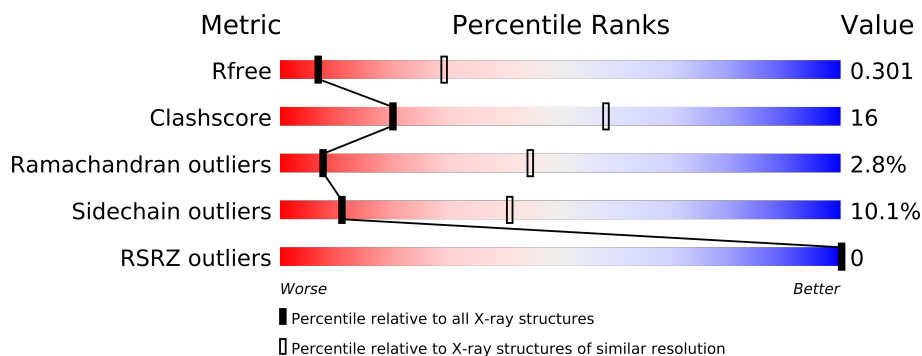
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	212	
1	L	212	
2	C	223	
2	H	223	
3	A	214	
3	D	214	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	3371	-	X
4	NAG	A	4201	-	X
4	NAG	D	3371	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Matuzumab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1533	959	252	316	6			
1	B	175	Total	C	N	O	S	0	0	0
			1239	772	204	258	5			

- Molecule 2 is a protein called Matuzumab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1573	996	259	311	7			
2	C	191	Total	C	N	O	S	0	0	0
			1347	846	224	270	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	191	Total	C	N	O	S	0	0	0
			1371	857	237	269	8			
3	D	191	Total	C	N	O	S	0	0	0
			1296	807	226	255	8			

There are 22 discrepancies between the modelled and reference sequences:

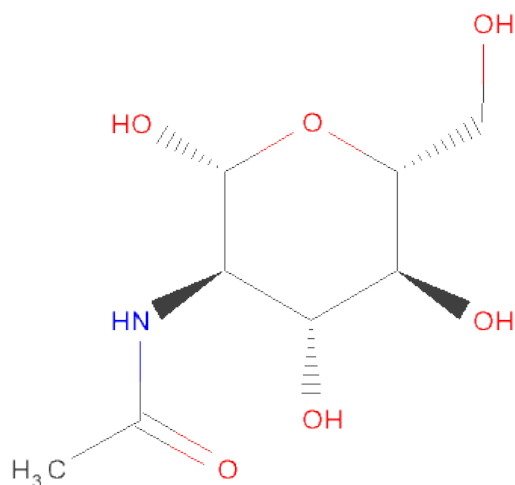
Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	EXPRESSION TAG	UNP P00533
A	308	GLU	-	EXPRESSION TAG	UNP P00533
A	309	GLU	-	EXPRESSION TAG	UNP P00533
A	310	LYS	-	EXPRESSION TAG	UNP P00533
A	311	LYS	-	EXPRESSION TAG	UNP P00533
A	515	HIS	-	EXPRESSION TAG	UNP P00533
A	516	HIS	-	EXPRESSION TAG	UNP P00533
A	517	HIS	-	EXPRESSION TAG	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
A	518	HIS	-	EXPRESSION TAG	UNP P00533
A	519	HIS	-	EXPRESSION TAG	UNP P00533
A	520	HIS	-	EXPRESSION TAG	UNP P00533
D	307	LEU	-	EXPRESSION TAG	UNP P00533
D	308	GLU	-	EXPRESSION TAG	UNP P00533
D	309	GLU	-	EXPRESSION TAG	UNP P00533
D	310	LYS	-	EXPRESSION TAG	UNP P00533
D	311	LYS	-	EXPRESSION TAG	UNP P00533
D	515	HIS	-	EXPRESSION TAG	UNP P00533
D	516	HIS	-	EXPRESSION TAG	UNP P00533
D	517	HIS	-	EXPRESSION TAG	UNP P00533
D	518	HIS	-	EXPRESSION TAG	UNP P00533
D	519	HIS	-	EXPRESSION TAG	UNP P00533
D	520	HIS	-	EXPRESSION TAG	UNP P00533

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



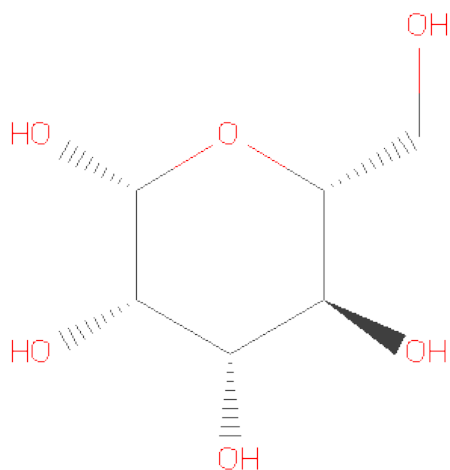
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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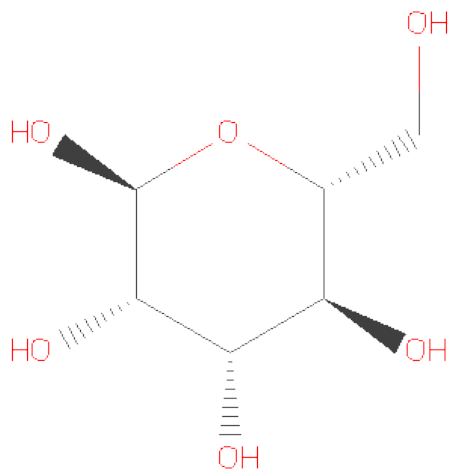
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



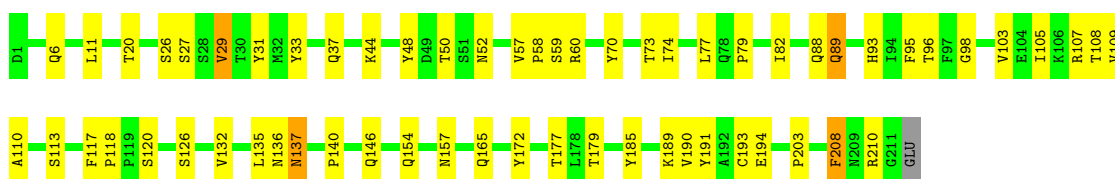
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

### 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.

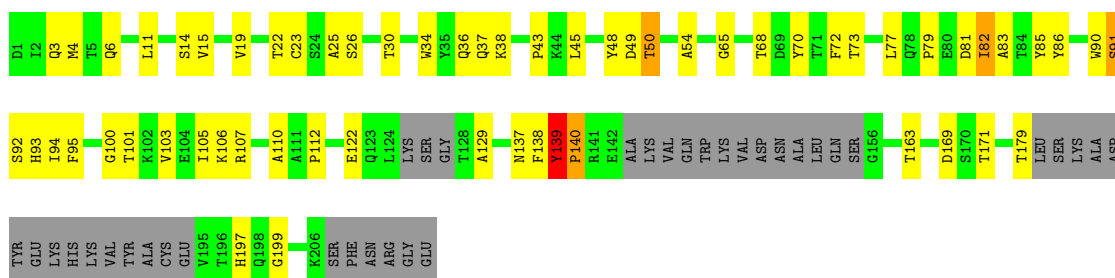
- Molecule 1: Matuzumab Fab Light chain

Chain L: 



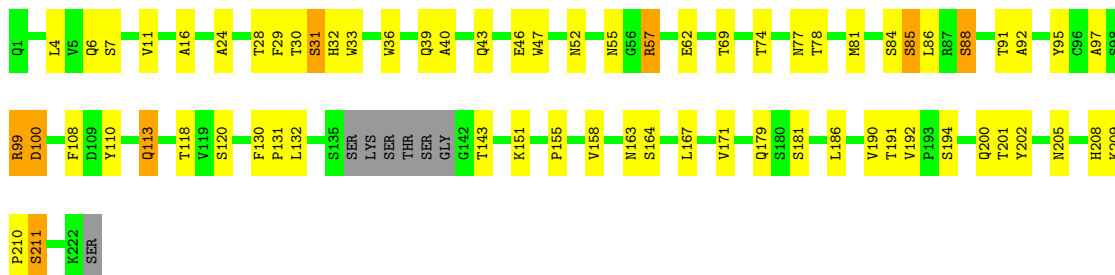
- Molecule 1: Matuzumab Fab Light chain

Chain B: 



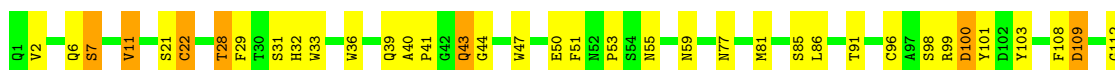
- Molecule 2: Matuzumab Fab Heavy chain

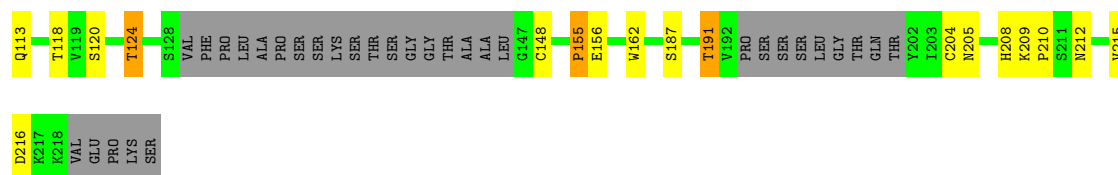
Chain H: 



- Molecule 2: Matuzumab Fab Heavy chain

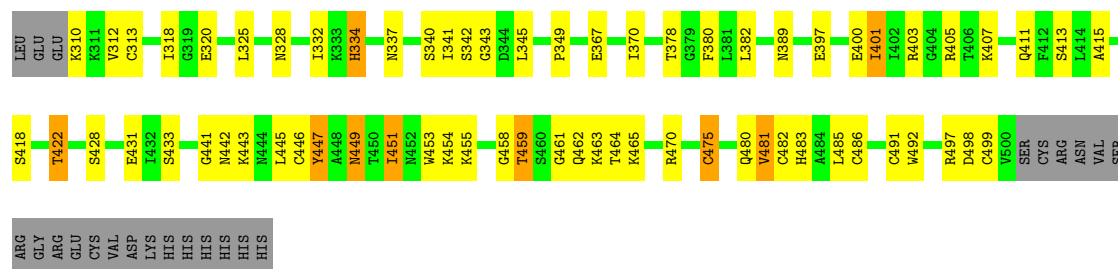
Chain C: 





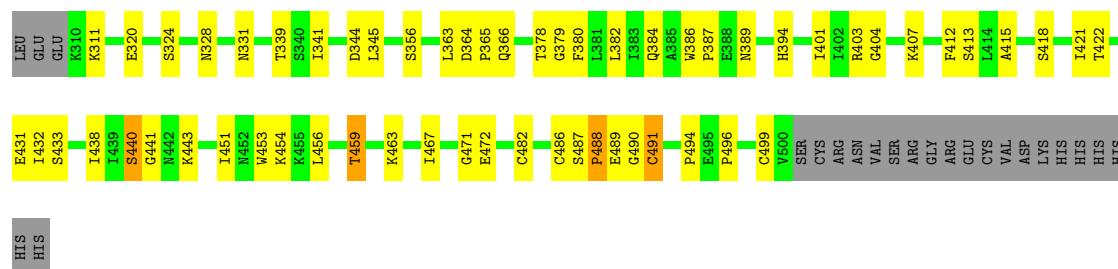
• Molecule 3: Epidermal growth factor receptor

Chain A: 



• Molecule 3: Epidermal growth factor receptor

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.07Å 205.03Å 81.58Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	36.56 – 3.20 45.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.56-3.20) 99.7 (45.47-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.242 , 0.299 0.241 , 0.301	Depositor DCC
$R_{free}$ test set	1709 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 18.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 33738 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, MAN

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	B	0.51	1/1266 (0.1%)	0.66	1/1732 (0.1%)
1	L	0.48	0/1570	0.63	0/2152
2	C	0.49	0/1383	0.63	0/1902
2	H	0.49	0/1616	0.61	0/2223
3	A	0.46	0/1396	0.64	0/1907
3	D	0.46	0/1322	0.60	0/1815
All	All	0.48	1/8553 (0.0%)	0.63	1/11731 (0.0%)

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
2	C	0	1
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	CYS	CB-SG	-5.02	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	TYR	C-N-CD	-5.46	108.59	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	191	THR	Peptide
2	H	99	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1239	0	1067	56	0
1	L	1533	0	1358	47	0
2	C	1347	0	1109	36	0
2	H	1573	0	1405	39	0
3	A	1371	0	1271	48	0
3	D	1296	0	1101	33	0
4	A	84	0	78	10	0
4	D	56	0	52	4	0
5	A	11	0	10	1	0
5	D	11	0	10	0	0
6	A	11	0	10	1	0
All	All	8532	0	7471	243	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 243 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:TYR:CD2	1:B:140:PRO:HD3	1.69	1.26
1:B:139:TYR:CG	1:B:140:PRO:HD3	1.74	1.22
1:B:139:TYR:CB	1:B:140:PRO:CD	2.27	1.10
1:B:139:TYR:HB3	1:B:140:PRO:CD	1.82	1.09
1:B:139:TYR:CG	1:B:140:PRO:CD	2.41	1.03

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	B	167/212 (79%)	145 (87%)	16 (10%)	6 (4%)	5	36
1	L	209/212 (99%)	189 (90%)	15 (7%)	5 (2%)	9	51
2	C	185/223 (83%)	159 (86%)	21 (11%)	5 (3%)	8	46
2	H	212/223 (95%)	190 (90%)	17 (8%)	5 (2%)	9	51
3	A	189/214 (88%)	153 (81%)	32 (17%)	4 (2%)	11	55
3	D	189/214 (88%)	153 (81%)	29 (15%)	7 (4%)	5	34
All	All	1151/1298 (89%)	989 (86%)	130 (11%)	32 (3%)	8	44

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	50	THR
1	B	122	GLU
1	B	139	TYR
1	B	140	PRO
2	H	30	THR

### 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	B	124/188 (66%)	115 (93%)	9 (7%)	20	62
1	L	158/188 (84%)	146 (92%)	12 (8%)	19	60
2	C	122/190 (64%)	106 (87%)	16 (13%)	6	28
2	H	159/190 (84%)	139 (87%)	20 (13%)	7	30
3	A	142/188 (76%)	125 (88%)	17 (12%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	118/188 (63%)	109 (92%)	9 (8%)	19	60
All	All	823/1132 (73%)	740 (90%)	83 (10%)	11	41

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	401	ILE
3	A	475	CYS
3	D	356	SER
3	A	411	GLN
3	A	451	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	337	ASN
3	A	480	GLN
3	D	384	GLN
3	A	462	GLN
3	A	483	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 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	3281	-	12,14,15	0.85	1 (8%)	15,19,21	1.46	3 (20%)
4	NAG	A	3282	-	12,14,15	0.81	1 (8%)	15,19,21	1.47	3 (20%)
5	BMA	A	3283	-	10,11,12	0.54	0	11,15,17	0.75	0
6	MAN	A	3284	-	10,11,12	0.69	0	11,15,17	0.75	0
4	NAG	A	3371	-	12,14,15	0.60	0	15,19,21	1.85	2 (13%)
4	NAG	A	3891	-	12,14,15	0.66	0	15,19,21	1.08	1 (6%)
4	NAG	A	4201	-	12,14,15	0.75	0	15,19,21	1.54	2 (13%)
4	NAG	A	4202	-	12,14,15	0.60	0	15,19,21	1.16	1 (6%)
4	NAG	D	3281	-	12,14,15	0.72	0	15,19,21	1.68	3 (20%)
4	NAG	D	3282	-	12,14,15	0.69	0	15,19,21	1.59	2 (13%)
5	BMA	D	3283	-	10,11,12	0.60	0	11,15,17	1.82	3 (27%)
4	NAG	D	3371	-	12,14,15	0.55	0	15,19,21	0.74	0
4	NAG	D	3891	-	12,14,15	0.64	0	15,19,21	0.64	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
4	NAG	A	3281	-	-	0/6/23/26	0/1/1/1
4	NAG	A	3282	-	-	0/6/23/26	0/1/1/1
5	BMA	A	3283	-	-	0/2/19/22	0/1/1/1
6	MAN	A	3284	-	-	0/2/19/22	0/1/1/1
4	NAG	A	3371	-	-	0/6/23/26	0/1/1/1
4	NAG	A	3891	-	-	0/6/23/26	0/1/1/1
4	NAG	A	4201	-	-	0/6/23/26	0/1/1/1
4	NAG	A	4202	-	-	0/6/23/26	0/1/1/1
4	NAG	D	3281	-	-	0/6/23/26	0/1/1/1
4	NAG	D	3282	-	-	0/6/23/26	0/1/1/1
5	BMA	D	3283	-	-	0/2/19/22	0/1/1/1
4	NAG	D	3371	-	-	0/6/23/26	0/1/1/1
4	NAG	D	3891	-	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3281	NAG	O5-C5	-2.40	1.40	1.45
4	A	3282	NAG	O5-C5	-2.19	1.41	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3371	NAG	O5-C5-C4	4.72	116.64	110.65
4	A	4201	NAG	C3-C4-C5	4.41	118.08	110.20
4	A	3371	NAG	C3-C4-C5	4.36	117.99	110.20
5	D	3283	BMA	C3-C4-C5	4.19	117.68	110.20
4	A	3281	NAG	C3-C4-C5	3.63	116.68	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	B	175/212 (82%)	-0.09	0 100 100	27, 40, 96, 100	0
1	L	211/212 (99%)	-0.28	0 100 100	25, 42, 73, 83	0
2	C	191/223 (85%)	-0.19	0 100 100	34, 51, 81, 83	0
2	H	216/223 (96%)	-0.23	0 100 100	31, 50, 63, 69	0
3	A	191/214 (89%)	-0.29	0 100 100	34, 47, 76, 81	0
3	D	191/214 (89%)	-0.28	0 100 100	44, 53, 89, 94	0
All	All	1175/1298 (90%)	-0.23	0 100 100	25, 49, 82, 100	0

There are no RSRZ outliers to report.

### 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 ⓘ

There are no carbohydrates in this entry.

### 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	4201	14/15	0.23	2.82	76,78,78,78	0
4	NAG	D	3371	14/15	0.26	2.09	104,106,106,107	0
4	NAG	A	3371	14/15	0.22	2.07	82,85,85,86	0
4	NAG	A	3282	14/15	0.22	0.88	52,54,55,57	0
4	NAG	A	3281	14/15	0.20	-0.09	31,35,42,42	0
4	NAG	D	3282	14/15	0.15	-0.54	67,70,73,74	0
4	NAG	D	3281	14/15	0.16	-0.69	33,37,39,41	0
6	MAN	A	3284	11/12	0.20	-	91,94,95,95	0
5	BMA	A	3283	11/12	0.26	-	108,108,108,109	0
5	BMA	D	3283	11/12	0.20	-	111,112,112,112	0
4	NAG	A	4202	14/15	0.43	-	102,103,103,103	0
4	NAG	D	3891	14/15	0.23	-	96,97,98,98	0
4	NAG	A	3891	14/15	0.18	-	99,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.