



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2016 – 08:10 AM EDT

PDB ID : 5I5K  
Title : Structure of complement C5 in complex with eculizumab  
Authors : Schatz-Jakobsen, J.A.; Andersen, G.R.  
Deposited on : 2016-02-15  
Resolution : 4.20 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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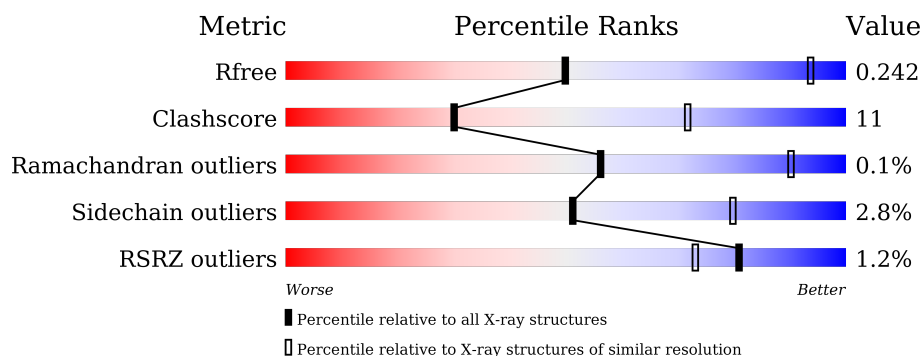
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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-20027790

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## X-RAY DIFFRACTION

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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1676	<div><div></div><div></div><div></div></div> %	<div><div></div><div></div><div></div></div> 71% 25% ..
1	B	1676	<div><div></div><div></div><div></div></div>	<div><div></div><div></div><div></div></div> 70% 27% ..
2	H	230	<div><div></div><div></div><div></div></div> %	<div><div></div><div></div><div></div></div> 70% 26% ..
2	X	230	<div><div></div><div></div><div></div></div> 3%	<div><div></div><div></div><div></div></div> 64% 31% . .
3	L	214	<div><div></div><div></div><div></div></div> 2%	<div><div></div><div></div><div></div></div> 71% 28%
3	Y	214	<div><div></div><div></div><div></div></div> 7%	<div><div></div><div></div><div></div></div> 70% 29%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32530 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1634	Total	C	N	O	S	0	0	0
			12932	8277	2126	2476	53			
1	A	1632	Total	C	N	O	S	0	0	0
			12922	8271	2124	2474	53			

- Molecule 2 is a protein called Eculizumab heavy chain (variable domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1679	1064	276	332	7			
2	X	221	Total	C	N	O	S	0	0	0
			1679	1064	276	332	7			

- Molecule 3 is a protein called Eculizumab light chain (variable domain).

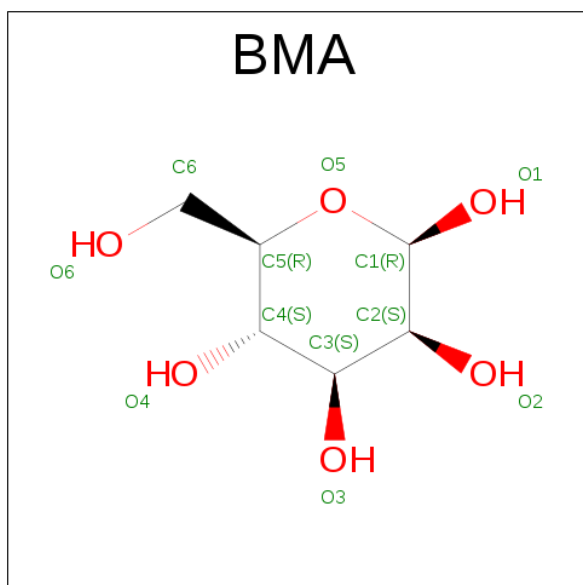
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1620	1013	270	332	5			
3	Y	213	Total	C	N	O	S	0	0	0
			1620	1013	270	332	5			

- Molecule 4 is 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	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	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		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).

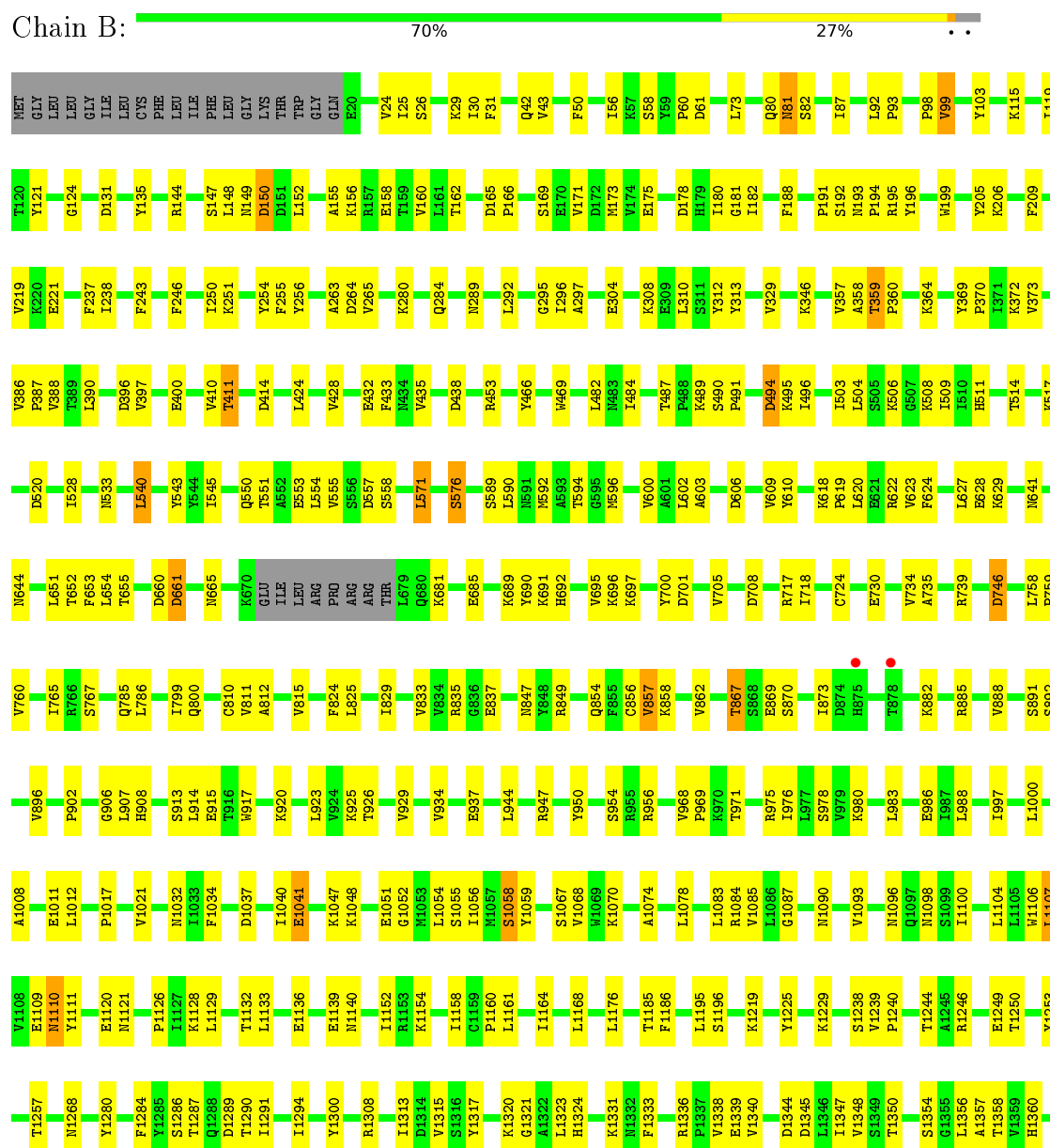


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

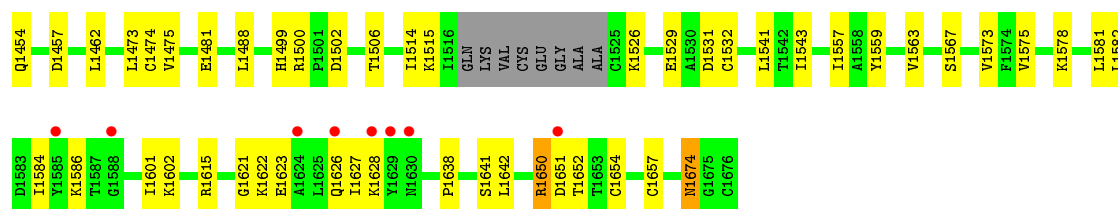
### 3 Residue-property plots

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.

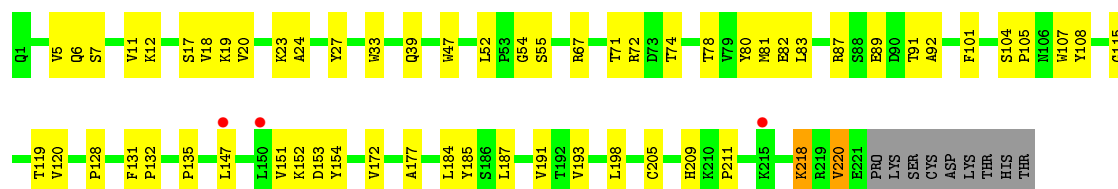
#### • Molecule 1: Complement C5



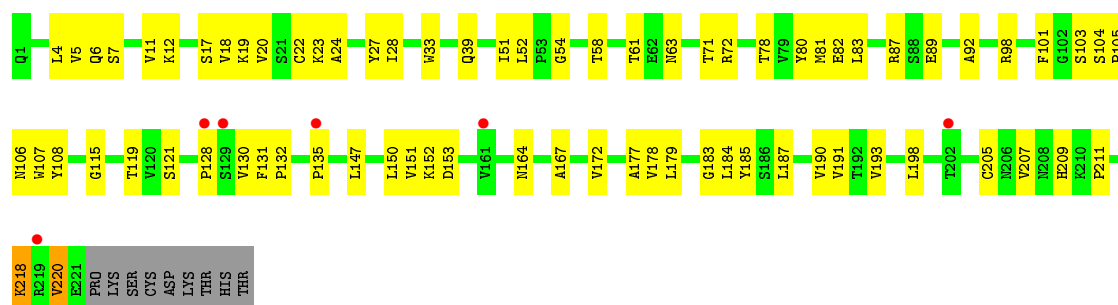




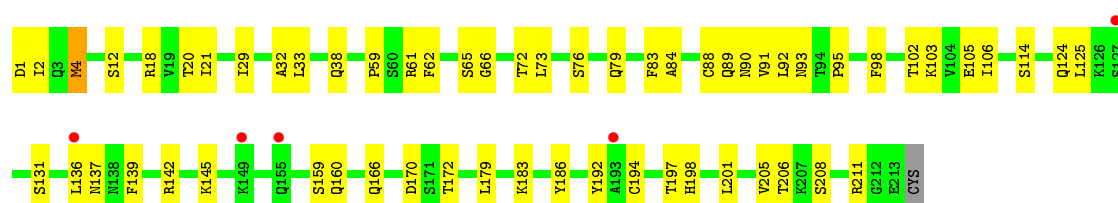
• Molecule 2: Eculizumab heavy chain (variable domain)



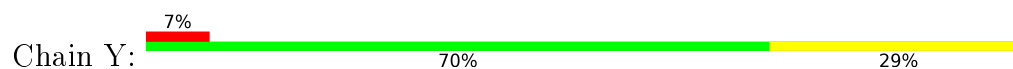
• Molecule 2: Eculizumab heavy chain (variable domain)



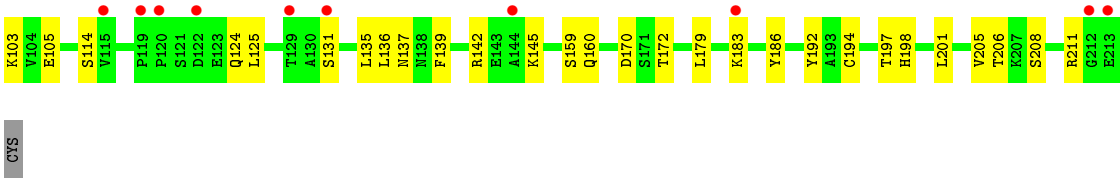
• Molecule 3: Eculizumab light chain (variable domain)



• Molecule 3: Eculizumab light chain (variable domain)







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.70Å 269.32Å 202.82Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	49.80 – 4.20 49.79 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.80-4.20) 99.7 (49.79-4.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10 _2152: ???)	Depositor
R, $R_{free}$	0.204 , 0.244 0.203 , 0.242	Depositor DCC
$R_{free}$ test set	1863 reflections (2.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	182.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 161.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	244.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.27	1/13201 (0.0%)	0.46	0/17907
1	B	0.27	1/13211 (0.0%)	0.46	1/17921 (0.0%)
2	H	0.26	0/1723	0.51	0/2350
2	X	0.26	0/1723	0.51	0/2350
3	L	0.26	0/1653	0.49	1/2247 (0.0%)
3	Y	0.26	0/1653	0.49	1/2247 (0.0%)
All	All	0.27	2/33164 (0.0%)	0.47	3/45022 (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
1	A	0	2
1	B	0	2
2	H	0	1
2	X	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	SER	C-N	10.24	1.53	1.34
1	B	576	SER	C-N	9.38	1.52	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	66	GLY	N-CA-C	5.42	126.66	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	66	GLY	N-CA-C	5.13	125.93	113.10
1	B	1107	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	LYS	Peptide
1	A	494	ASP	Peptide
1	B	489	LYS	Peptide
1	B	494	ASP	Peptide
2	H	108	TYR	Peptide

## 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	12922	0	12866	277	0
1	B	12932	0	12876	289	0
2	H	1679	0	1628	42	0
2	X	1679	0	1628	48	0
3	L	1620	0	1576	41	0
3	Y	1620	0	1576	39	0
4	A	28	0	24	1	0
4	B	28	0	24	1	0
5	A	11	0	10	0	0
5	B	11	0	10	0	0
All	All	32530	0	32218	717	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 11.

The worst 5 of 717 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:B:1106:TRP:O	1:B:1110:ASN:HB2	1.48	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:TRP:O	1:A:1110:ASN:HB2	1.49	1.09
1:A:364:LYS:NZ	1:A:557:ASP:OD2	1.85	1.07
1:B:1229:LYS:HZ1	1:B:1240:PRO:HD2	1.28	0.96
1:A:150:ASP:OD2	1:A:508:LYS:NZ	2.00	0.94

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	1624/1676 (97%)	1552 (96%)	70 (4%)	2 (0%)	56	90
1	B	1626/1676 (97%)	1553 (96%)	71 (4%)	2 (0%)	56	90
2	H	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
2	X	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
3	L	211/214 (99%)	197 (93%)	14 (7%)	0	100	100
3	Y	211/214 (99%)	196 (93%)	15 (7%)	0	100	100
All	All	4110/4240 (97%)	3913 (95%)	193 (5%)	4 (0%)	56	90

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1573	VAL
1	A	1573	VAL
1	B	1651	ASP
1	A	1651	ASP

### 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	1450/1484 (98%)	1406 (97%)	44 (3%)	48	79
1	B	1450/1484 (98%)	1406 (97%)	44 (3%)	48	79
2	H	190/199 (96%)	187 (98%)	3 (2%)	70	88
2	X	190/199 (96%)	187 (98%)	3 (2%)	70	88
3	L	184/185 (100%)	181 (98%)	3 (2%)	70	88
3	Y	184/185 (100%)	180 (98%)	4 (2%)	60	84
All	All	3648/3736 (98%)	3547 (97%)	101 (3%)	51	80

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	218	LYS
1	A	208	ASP
1	A	1674	ASN
3	L	4	MET
1	A	73	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	800	GLN
1	A	665	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	2001	1,4	14,14,15	0.66	0	15,19,21	0.38	0
4	NAG	A	2002	5,4	14,14,15	0.54	0	15,19,21	1.33	1 (6%)
5	BMA	A	2003	4	11,11,12	0.51	0	15,15,17	0.73	0
4	NAG	B	2001	1,4	14,14,15	0.56	0	15,19,21	0.32	0
4	NAG	B	2002	5,4	14,14,15	0.65	1 (7%)	15,19,21	1.25	1 (6%)
5	BMA	B	2003	4	11,11,12	0.58	0	15,15,17	0.70	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	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	2003	4	-	0/2/19/22	0/1/1/1
4	NAG	B	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	B	2003	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	NAG	C1-C2	2.22	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	NAG	C2-N2-C7	4.52	128.99	123.11
4	A	2002	NAG	C2-N2-C7	4.56	129.04	123.11

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
4	A	2002	NAG	1	0
4	B	2002	NAG	1	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

### 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	1632/1676 (97%)	-0.25	21 (1%) 79 71	120, 256, 409, 564	0
1	B	1634/1676 (97%)	-0.52	2 (0%) 95 95	122, 185, 271, 483	0
2	H	221/230 (96%)	-0.21	3 (1%) 78 69	177, 262, 403, 459	0
2	X	221/230 (96%)	-0.22	6 (2%) 58 47	207, 297, 454, 565	0
3	L	213/214 (99%)	-0.02	5 (2%) 64 53	181, 289, 424, 499	0
3	Y	213/214 (99%)	0.06	14 (6%) 22 15	183, 315, 423, 494	0
All	All	4134/4240 (97%)	-0.32	51 (1%) 81 73	120, 225, 399, 565	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	530	VAL	8.6
1	A	1630	ASN	8.2
1	A	1624	ALA	7.6
2	H	150	LEU	6.3
3	Y	212	GLY	6.0

### 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 [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
5	BMA	B	2003	11/12	0.86	0.15	-	188,266,294,295	0
4	NAG	B	2001	14/15	0.94	0.16	-	149,202,253,254	0
4	NAG	A	2002	14/15	0.86	0.24	-	220,281,316,337	0
4	NAG	B	2002	14/15	0.91	0.14	-	242,277,305,310	0
5	BMA	A	2003	11/12	0.85	0.35	-	302,324,338,340	0
4	NAG	A	2001	14/15	0.94	0.18	-	167,236,272,278	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.