



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:46 PM GMT

PDB ID : 4FXG  
Title : Complement C4 in complex with MASP-2  
Authors : Kidmose, R.T.; Laursen, N.S.; Andersen, G.R.  
Deposited on : 2012-07-03  
Resolution : 3.75 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

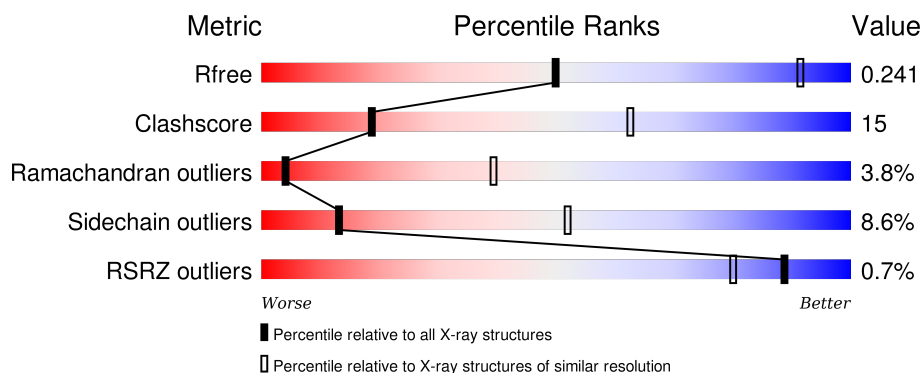
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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	656	<div> <div></div> <div>62%33% . .</div> </div>
1	D	656	<div> <div></div> <div>63%32% . .</div> </div>
2	B	767	<div> <div>1%</div> <div>57%35% . .</div> </div>
2	E	767	<div> <div>2%</div> <div>58%35% . .</div> </div>
3	C	291	<div> <div></div> <div>55%35%8% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	291	<div><div></div><div>59%31%8%</div><div></div></div>
4	G	154	<div><div></div><div>70%21%6%</div><div></div></div>
4	I	154	<div><div>%</div><div></div><div>71%20%6%</div><div></div></div>
5	H	242	<div><div>%</div><div></div><div>64%31%5%</div><div></div></div>
5	J	242	<div><div>%</div><div></div><div>64%31%5%</div><div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32218 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 C4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			
1	D	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			

- Molecule 2 is a protein called Complement C4-A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			
2	E	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			

- Molecule 3 is a protein called Complement C4 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	0	0	0
			2291	1437	407	430	17			
3	F	287	Total	C	N	O	S	0	0	0
			2291	1437	407	430	17			

- Molecule 4 is a protein called Mannan-binding lectin serine protease 2 A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			
4	I	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	298	HIS	GLN	CONFLICT	UNP O00187
G	299	ALA	PRO	CONFLICT	UNP O00187
I	298	HIS	GLN	CONFLICT	UNP O00187
I	299	ALA	PRO	CONFLICT	UNP O00187

- Molecule 5 is a protein called Mannan-binding lectin serine protease 2 B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	242	Total	C	N	O	S	0	0	0
			1868	1190	317	351	10			
5	J	242	Total	C	N	O	S	0	0	0
			1868	1190	317	351	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	633	ALA	SER	ENGINEERED MUTATION	UNP O00187
J	633	ALA	SER	ENGINEERED MUTATION	UNP O00187

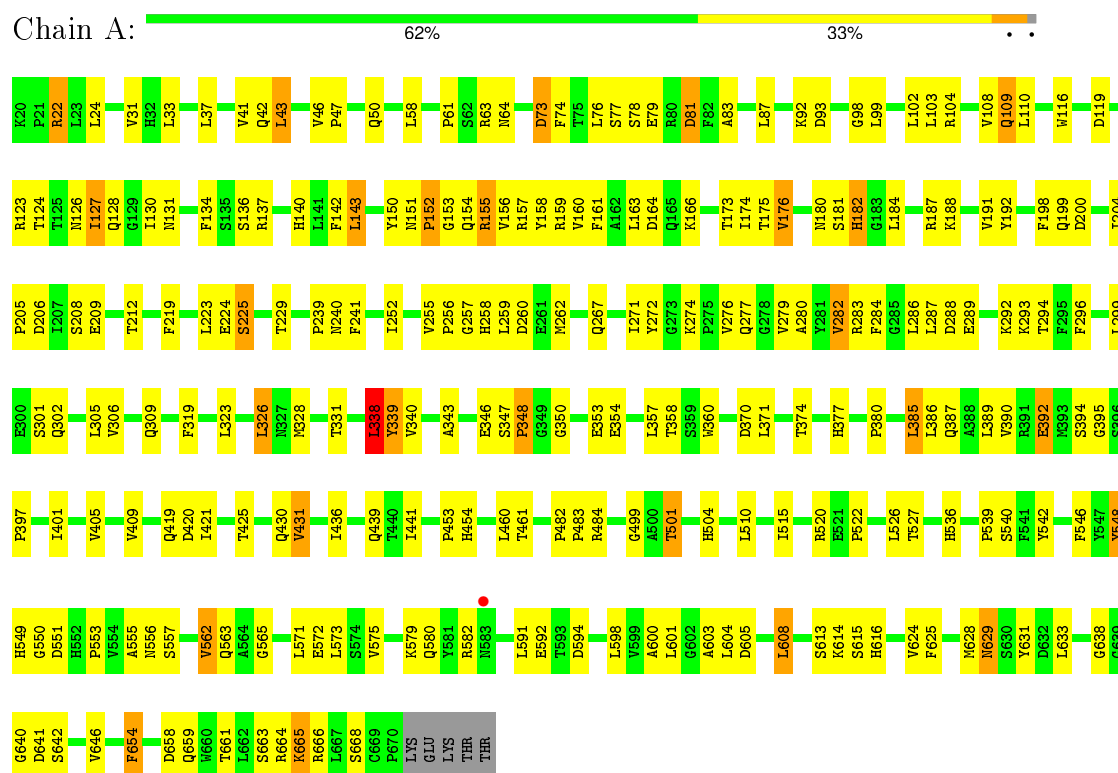
- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	B	3	Total	C	N	O	0	0
			39	22	2	15		
6	D	3	Total	C	N	O	0	0
			39	22	2	15		
6	B	3	Total	C	N	O	0	0
			39	22	2	15		
6	E	3	Total	C	N	O	0	0
			39	22	2	15		
6	E	3	Total	C	N	O	0	0
			39	22	2	15		

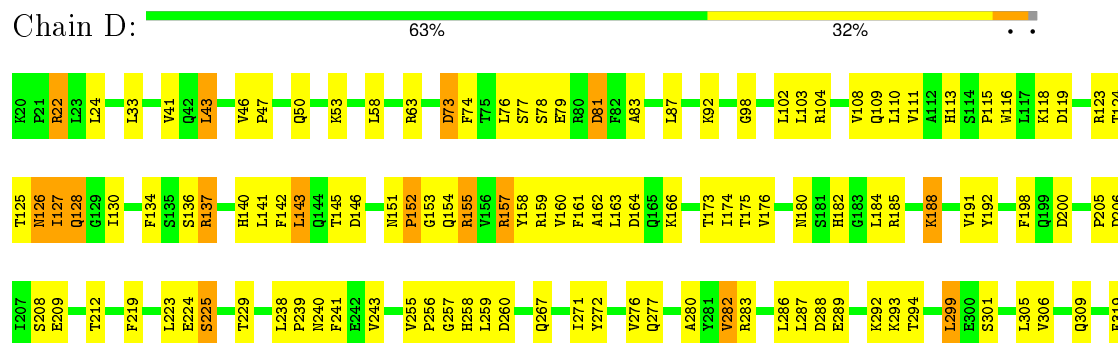
### 3 Residue-property plots

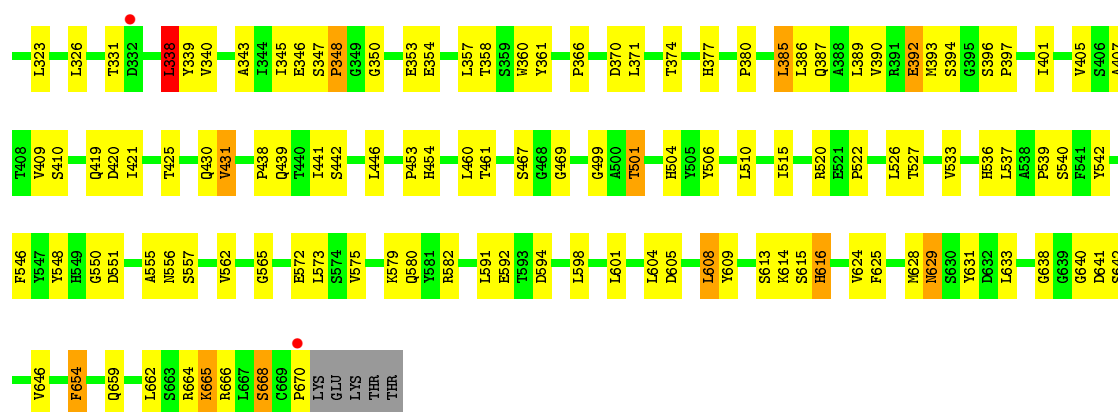
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 C4 beta chain

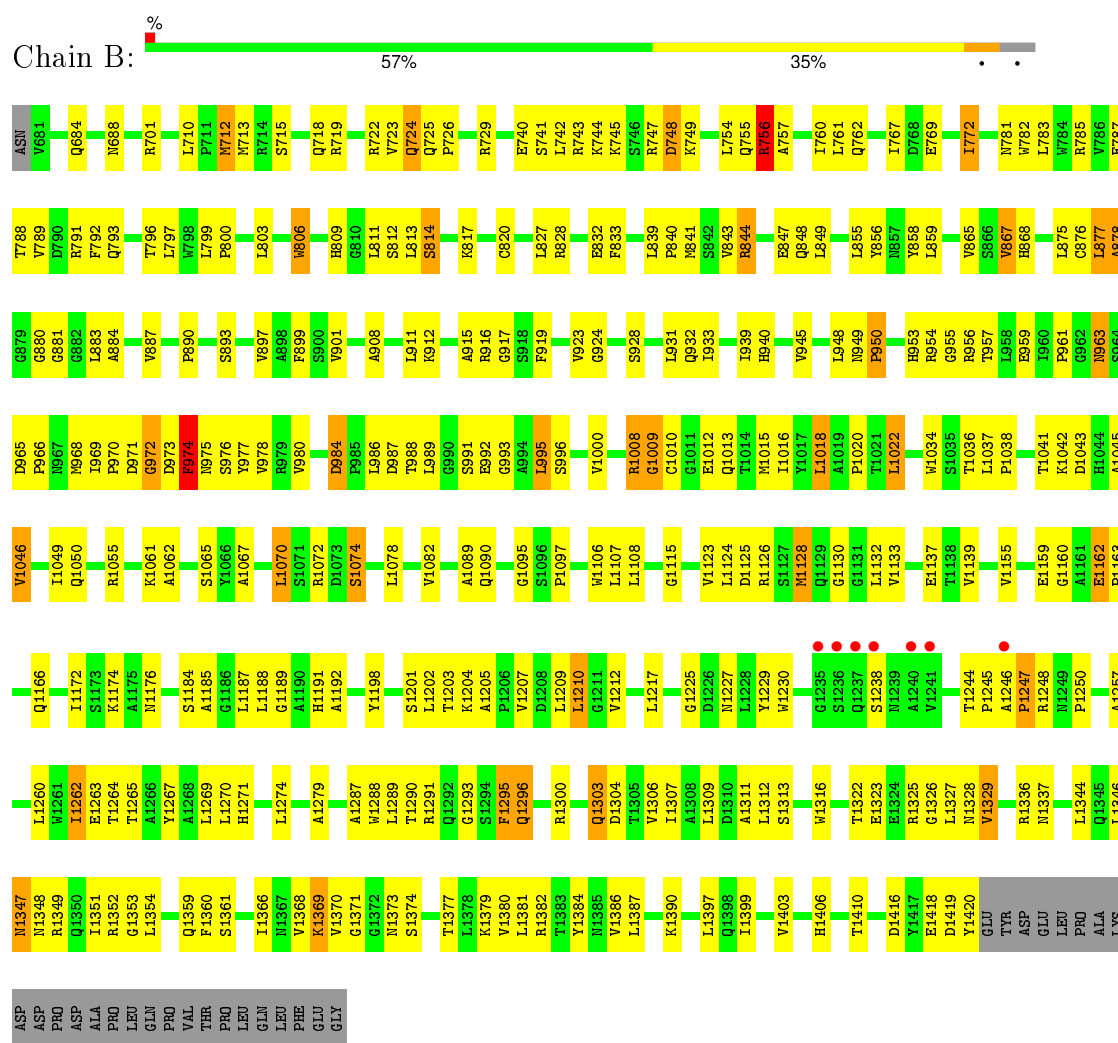


#### • Molecule 1: Complement C4 beta chain

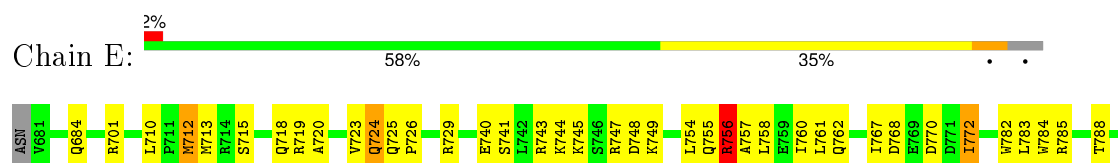


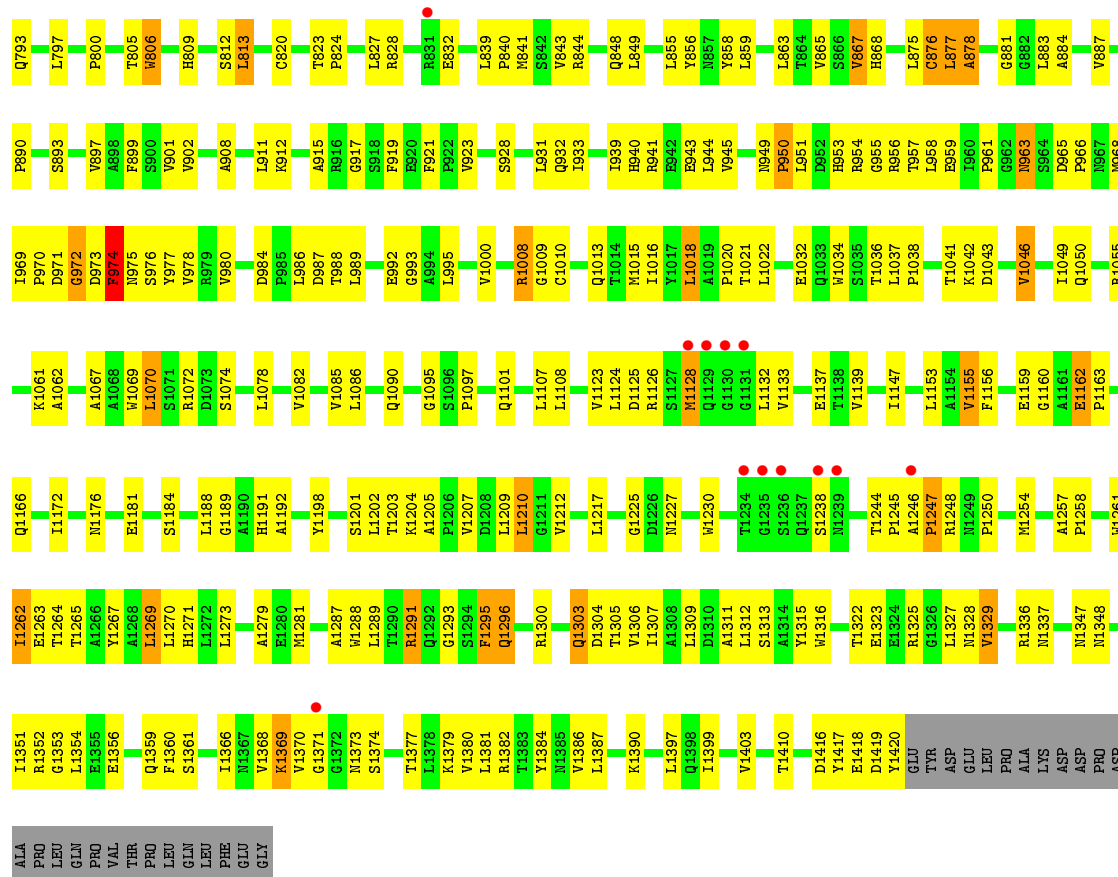


• Molecule 2: Complement C4-A alpha chain



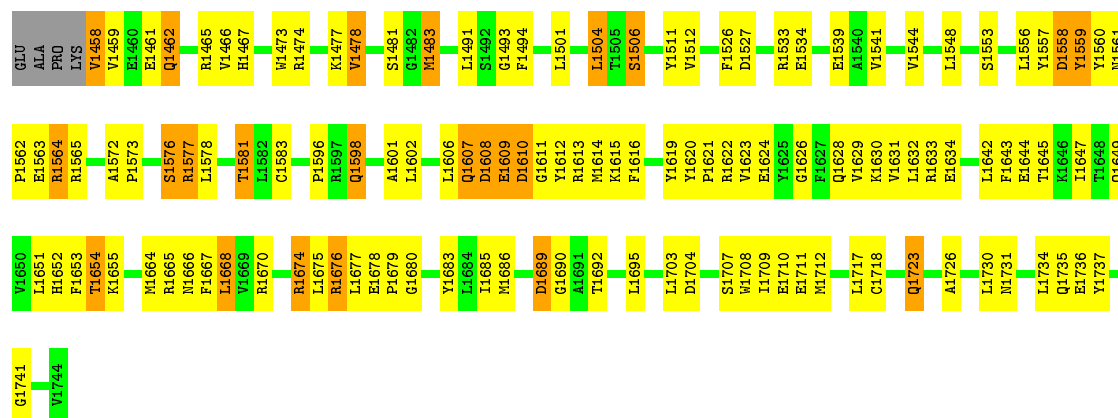
• Molecule 2: Complement C4-A alpha chain





• Molecule 3: Complement C4 gamma chain

Chain C: 55% 35% 8%

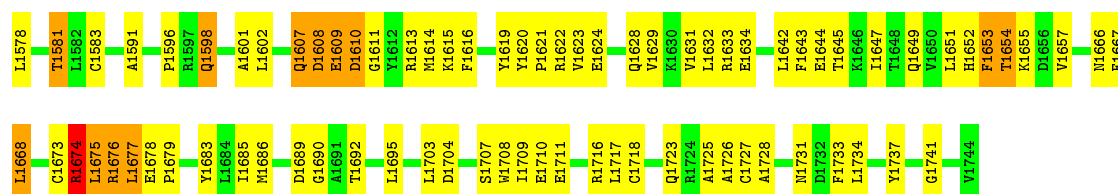


• Molecule 3: Complement C4 gamma chain

Chain F: 59% 31% 8%

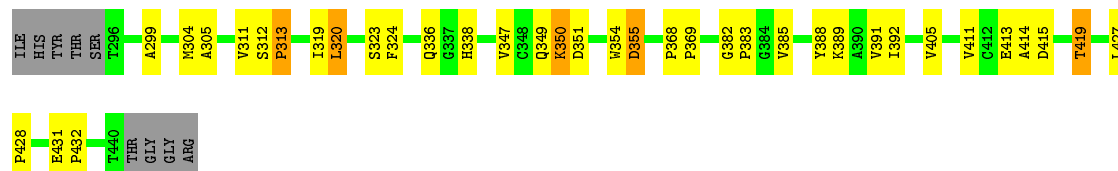






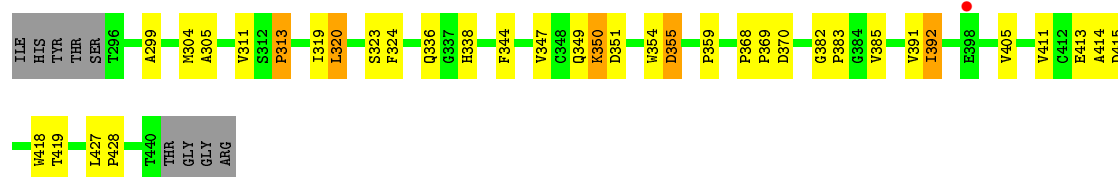
- Molecule 4: Mannan-binding lectin serine protease 2 A chain

Chain G: 70% 21% 6%



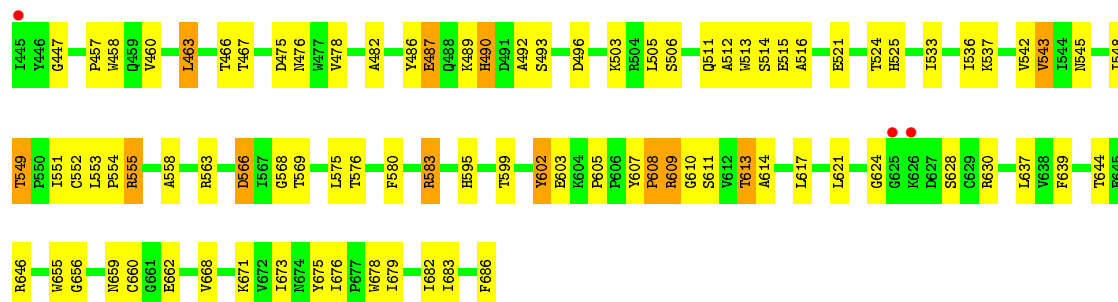
- Molecule 4: Mannan-binding lectin serine protease 2 A chain

Chain I: 71% 20% 6%



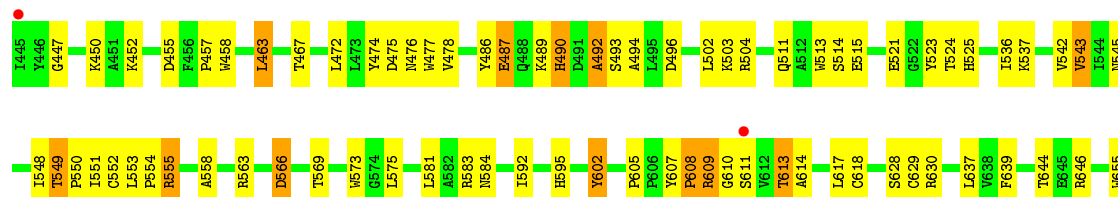
- Molecule 5: Mannan-binding lectin serine protease 2 B chain

Chain H: 64% 31% 5%



- Molecule 5: Mannan-binding lectin serine protease 2 B chain

Chain J: 64% 31% 5%



6656		6659		6660		6661		6662		6668		6671		6672		6673		6676		6679		6683		6686
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.01Å 215.01Å 142.86Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	48.97 – 3.75 48.97 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.97-3.75) 98.6 (48.97-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.174 , 0.241 0.174 , 0.241	Depositor DCC
$R_{free}$ test set	1726 reflections (3.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	118.2	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 66.6	EDS
Estimated twinning fraction	0.083 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 56608 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: BMA, NAG, TYS

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	0.31	0/5128	0.58	1/6961 (0.0%)
1	D	0.33	0/5128	0.58	1/6961 (0.0%)
2	B	0.32	0/5799	0.63	3/7875 (0.0%)
2	E	0.32	0/5799	0.61	2/7875 (0.0%)
3	C	0.35	0/2338	0.64	0/3158
3	F	0.35	0/2338	0.64	1/3158 (0.0%)
4	G	0.33	0/1136	0.60	0/1549
4	I	0.34	0/1136	0.60	0/1549
5	H	0.28	0/1916	0.50	0/2604
5	J	0.32	0/1916	0.53	0/2604
All	All	0.32	0/32634	0.60	8/44294 (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	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	756	ARG	NE-CZ-NH2	19.88	130.24	120.30
2	E	756	ARG	NE-CZ-NH2	16.11	128.36	120.30
2	B	756	ARG	NE-CZ-NH1	-9.44	115.58	120.30
2	E	756	ARG	NE-CZ-NH1	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	LEU	CA-CB-CG	6.03	129.17	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	SER	Peptide
1	D	225	SER	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	A	5012	0	5025	140	0
1	D	5012	0	5025	140	0
2	B	5718	0	5645	220	0
2	E	5718	0	5645	217	0
3	C	2291	0	2228	90	0
3	F	2291	0	2228	81	0
4	G	1103	0	1051	20	0
4	I	1103	0	1051	18	0
5	H	1868	0	1803	62	0
5	J	1868	0	1803	61	0
6	A	39	0	34	0	0
6	B	78	0	68	2	0
6	D	39	0	34	0	0
6	E	78	0	68	2	0
All	All	32218	0	31708	984	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 15.

The worst 5 of 984 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)
2:B:756:ARG:HG2	5:J:655:TRP:HA	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:756:ARG:HG2	5:H:655:TRP:HA	1.56	0.87
3:C:1631:VAL:HA	3:C:1645:THR:HG22	1.54	0.86
1:D:143:LEU:HB3	1:D:160:VAL:HG23	1.56	0.86
2:E:848:GLN:HE21	3:F:1548:LEU:HD22	1.43	0.83

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	649/656 (99%)	541 (83%)	88 (14%)	20 (3%)	5	45
1	D	649/656 (99%)	540 (83%)	89 (14%)	20 (3%)	5	45
2	B	737/767 (96%)	625 (85%)	84 (11%)	28 (4%)	4	39
2	E	737/767 (96%)	630 (86%)	81 (11%)	26 (4%)	4	42
3	C	285/291 (98%)	230 (81%)	41 (14%)	14 (5%)	3	32
3	F	285/291 (98%)	229 (80%)	43 (15%)	13 (5%)	3	34
4	G	143/154 (93%)	122 (85%)	13 (9%)	8 (6%)	2	29
4	I	143/154 (93%)	123 (86%)	12 (8%)	8 (6%)	2	29
5	H	240/242 (99%)	202 (84%)	29 (12%)	9 (4%)	4	39
5	J	240/242 (99%)	203 (85%)	28 (12%)	9 (4%)	4	39
All	All	4108/4220 (97%)	3445 (84%)	508 (12%)	155 (4%)	4	39

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	SER
2	B	878	ALA
2	B	950	PRO

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Mol	Chain	Res	Type
2	B	1132	LEU
2	B	1204	LYS

### 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	557/562 (99%)	504 (90%)	53 (10%)	11	46
1	D	557/562 (99%)	505 (91%)	52 (9%)	11	48
2	B	615/639 (96%)	558 (91%)	57 (9%)	11	48
2	E	615/639 (96%)	561 (91%)	54 (9%)	12	50
3	C	246/249 (99%)	222 (90%)	24 (10%)	10	44
3	F	246/249 (99%)	225 (92%)	21 (8%)	13	52
4	G	124/131 (95%)	119 (96%)	5 (4%)	38	75
4	I	124/131 (95%)	119 (96%)	5 (4%)	38	75
5	H	193/193 (100%)	179 (93%)	14 (7%)	17	58
5	J	193/193 (100%)	179 (93%)	14 (7%)	17	58
All	All	3470/3548 (98%)	3171 (91%)	299 (9%)	13	52

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	43	LEU
1	D	385	LEU
5	H	583	ARG
1	D	78	SER
1	D	182	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	949	ASN

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Mol	Chain	Res	Type
3	C	1700	GLN
2	E	848	GLN
2	B	848	GLN
2	E	684	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
2	TYS	B	1417	2	15,16,17	1.13	2 (13%)	16,22,24	1.38	1 (6%)
2	TYS	B	1420	-	15,16,17	0.93	1 (6%)	16,22,24	0.88	1 (6%)
2	TYS	E	1417	2	15,16,17	1.02	1 (6%)	16,22,24	1.64	4 (25%)
2	TYS	E	1420	-	15,16,17	0.91	2 (13%)	16,22,24	0.91	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
2	TYS	B	1417	2	-	0/9/11/13	0/1/1/1
2	TYS	B	1420	-	-	0/9/11/13	0/1/1/1
2	TYS	E	1417	2	-	0/9/11/13	0/1/1/1
2	TYS	E	1420	-	-	0/9/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1420	TYS	OH-CZ	-2.02	1.39	1.42
2	E	1417	TYS	OH-S	2.09	1.67	1.63
2	B	1417	TYS	CE1-CD1	2.21	1.42	1.38
2	E	1420	TYS	OH-S	2.51	1.68	1.63
2	B	1420	TYS	OH-S	2.62	1.68	1.63

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1417	TYS	OH-CZ-CE2	-2.69	113.42	118.74
2	E	1417	TYS	CZ-OH-S	-2.29	114.61	118.52
2	E	1420	TYS	OH-CZ-CE2	2.18	123.05	118.74
2	B	1420	TYS	OH-CZ-CE2	2.28	123.24	118.74
2	E	1417	TYS	CG-CB-CA	2.33	119.48	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1420	TYS	1	0
2	E	1417	TYS	1	0
2	E	1420	TYS	1	0

## 5.5 Carbohydrates ⓘ

18 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	701	1,6	14,14,15	0.95	1 (7%)	15,19,21	1.70	5 (33%)
6	NAG	A	702	6	14,14,15	0.59	0	15,19,21	1.13	1 (6%)
6	BMA	A	703	6	11,11,12	0.54	0	14,15,17	0.92	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	1501	2,6	14,14,15	1.11	0	15,19,21	3.38	8 (53%)
6	NAG	B	1502	6	14,14,15	1.11	1 (7%)	15,19,21	3.48	8 (53%)
6	BMA	B	1503	6	11,11,12	1.28	2 (18%)	14,15,17	2.02	6 (42%)
6	NAG	B	1504	2,6	14,14,15	0.56	0	15,19,21	0.85	0
6	NAG	B	1505	6	14,14,15	0.52	0	15,19,21	0.80	0
6	BMA	B	1506	6	11,11,12	0.59	0	14,15,17	0.69	0
6	NAG	D	701	1,6	14,14,15	0.91	1 (7%)	15,19,21	1.74	4 (26%)
6	NAG	D	702	6	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
6	BMA	D	703	6	11,11,12	0.55	0	14,15,17	0.77	0
6	NAG	E	1501	2,6	14,14,15	1.59	3 (21%)	15,19,21	4.03	11 (73%)
6	NAG	E	1502	6	14,14,15	1.19	1 (7%)	15,19,21	3.84	7 (46%)
6	BMA	E	1503	6	11,11,12	1.35	2 (18%)	14,15,17	3.21	6 (42%)
6	NAG	E	1504	2,6	14,14,15	0.57	0	15,19,21	1.00	0
6	NAG	E	1505	6	14,14,15	0.52	0	15,19,21	0.78	0
6	BMA	E	1506	6	11,11,12	0.59	0	14,15,17	0.71	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	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	702	6	-	0/6/23/26	0/1/1/1
6	BMA	A	703	6	-	0/2/19/22	0/1/1/1
6	NAG	B	1501	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1502	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1503	6	-	0/2/19/22	0/1/1/1
6	NAG	B	1504	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1505	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1506	6	-	0/2/19/22	0/1/1/1
6	NAG	D	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	702	6	-	0/6/23/26	0/1/1/1
6	BMA	D	703	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1501	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1502	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1503	6	-	0/2/19/22	0/1/1/1
6	NAG	E	1504	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1505	6	-	0/6/23/26	0/1/1/1
6	BMA	E	1506	6	-	0/2/19/22	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1502	NAG	O5-C1	-2.76	1.39	1.43
6	A	701	NAG	O5-C1	-2.68	1.39	1.43
6	E	1501	NAG	O5-C1	-2.59	1.39	1.43
6	D	701	NAG	O5-C1	-2.42	1.39	1.43
6	B	1502	NAG	O5-C1	-2.39	1.39	1.43

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1501	NAG	C2-N2-C7	-8.83	111.69	123.04
6	B	1501	NAG	C2-N2-C7	-8.53	112.08	123.04
6	B	1502	NAG	C2-N2-C7	-6.13	115.16	123.04
6	E	1501	NAG	O3-C3-C4	-5.05	98.96	110.34
6	B	1502	NAG	O3-C3-C2	-4.54	100.13	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1504	NAG	2	0
6	E	1504	NAG	2	0

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	651/656 (99%)	-0.39	1 (0%) 95 91	68, 116, 172, 203	0
1	D	651/656 (99%)	-0.39	2 (0%) 94 89	54, 103, 169, 213	0
2	B	738/767 (96%)	-0.34	7 (0%) 85 74	51, 109, 185, 245	0
2	E	738/767 (96%)	-0.25	12 (1%) 74 59	66, 114, 202, 290	0
3	C	287/291 (98%)	-0.48	0 100 100	52, 89, 137, 180	0
3	F	287/291 (98%)	-0.37	0 100 100	59, 92, 150, 193	0
4	G	145/154 (94%)	-0.54	0 100 100	89, 123, 167, 197	0
4	I	145/154 (94%)	-0.31	1 (0%) 89 80	86, 123, 186, 204	0
5	H	242/242 (100%)	-0.01	3 (1%) 81 67	117, 178, 222, 247	0
5	J	242/242 (100%)	-0.29	2 (0%) 87 77	77, 129, 183, 202	0
All	All	4126/4220 (97%)	-0.33	28 (0%) 89 80	51, 112, 190, 290	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1128	MET	3.9
2	B	1236	SER	3.8
2	B	1238	SER	3.7
2	E	1246	ALA	3.7
2	B	1246	ALA	3.6

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
2	TYS	E	1420	16/17	0.64	0.30	-	173,250,270,277	4
2	TYS	B	1417	16/17	0.72	0.33	-	114,210,238,244	4
2	TYS	E	1417	16/17	0.69	0.47	-	132,258,279,279	4
2	TYS	B	1420	16/17	0.73	0.35	-	209,229,236,239	4

### 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( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	1504	14/15	0.85	0.32	0.80	227,232,239,241	0
6	NAG	E	1504	14/15	0.83	0.26	-0.64	186,197,224,226	0
6	NAG	A	701	14/15	0.77	0.31	-	174,184,212,218	0
6	NAG	B	1501	14/15	0.93	0.31	-	214,224,238,245	0
6	BMA	A	703	11/12	0.85	0.19	-	159,171,177,179	0
6	BMA	E	1503	11/12	0.72	0.32	-	205,219,235,236	0
6	NAG	B	1505	14/15	0.75	0.30	-	209,215,234,239	0
6	NAG	B	1502	14/15	0.86	0.30	-	216,226,228,229	0
6	NAG	A	702	14/15	0.79	0.24	-	170,179,185,188	0
6	NAG	E	1502	14/15	0.82	0.30	-	213,218,243,245	0
6	BMA	D	703	11/12	0.77	0.25	-	233,241,247,252	0
6	NAG	E	1505	14/15	0.82	0.22	-	187,199,207,210	0
6	BMA	E	1506	11/12	0.78	0.20	-	182,195,199,203	0
6	BMA	B	1506	11/12	0.80	0.27	-	192,201,204,205	0
6	NAG	E	1501	14/15	0.91	0.22	-	197,205,224,225	0
6	BMA	B	1503	11/12	0.71	0.23	-	218,228,232,232	0
6	NAG	D	701	14/15	0.80	0.33	-	167,208,231,234	0
6	NAG	D	702	14/15	0.82	0.35	-	214,228,238,244	0

### 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.