



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:19 am GMT

PDB ID : 3WKN  
Title : Crystal structure of the artificial protein AFFinger p17 (AF.p17) complexed with Fc fragment of human IgG  
Authors : Watanabe, H.; Honda, S.  
Deposited on : 2013-10-29  
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

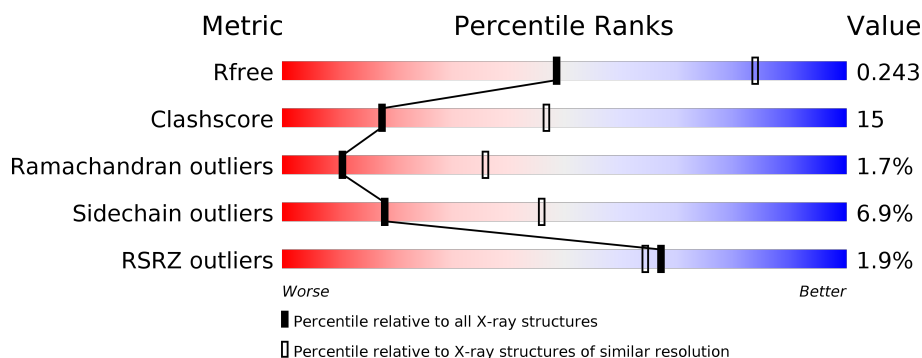
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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	212	<div> <div>66%</div> <div>30%</div> <div>• •</div> </div>
1	B	212	<div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
1	C	212	<div> <div>67%</div> <div>29%</div> <div>• •</div> </div>
1	D	212	<div> <div>63%</div> <div>33%</div> <div>• •</div> </div>
1	I	212	<div> <div>%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
1	J	212	<div> <div>%</div> <div>61%</div> <div>31%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	212	
1	N	212	
2	E	54	
2	F	54	
2	G	54	
2	H	54	
2	K	54	
2	L	54	
2	O	54	
2	P	54	

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
3	GAL	A	507	-	-	-	X
3	GAL	B	507	-	-	-	X
3	GAL	I	507	-	-	-	X
3	GAL	J	507	-	-	-	X
3	GAL	M	507	-	-	-	X
3	GAL	N	507	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17052 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	B	210	Total	C	N	O	S	0	0	0
			1675	1066	282	321	6			
1	A	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	D	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	I	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	J	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	M	209	Total	C	N	O	S	0	0	0
			1668	1061	281	320	6			
1	N	210	Total	C	N	O	S	0	0	0
			1675	1066	282	321	6			

- Molecule 2 is a protein called AFFinger p17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	29	Total	C	N	O	S	0	0	0
			250	163	39	47	1			
2	F	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	G	47	Total	C	N	O	S	0	0	0
			392	256	61	74	1			
2	H	32	Total	C	N	O	S	0	0	0
			274	180	42	51	1			
2	K	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	L	47	Total	C	N	O	S	0	0	0
			392	256	61	74	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	46	Total	C	N	O	S	0	0	0
			381	247	60	73	1			
2	P	43	Total	C	N	O	S	0	0	0
			363	236	57	69	1			

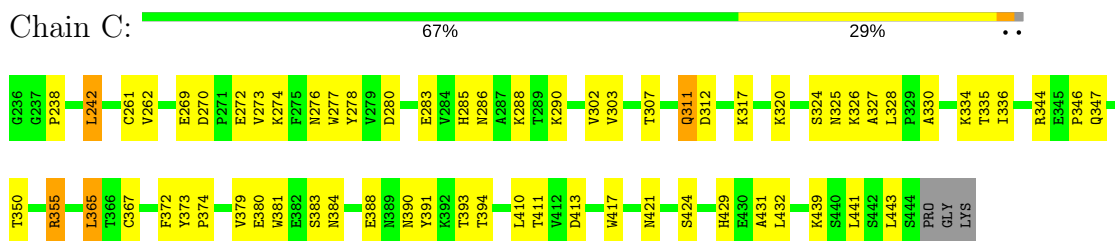
- Molecule 3 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	9	Total	C	N	O	0	0
			110	62	4	44		
3	B	9	Total	C	N	O	0	0
			110	62	4	44		
3	A	9	Total	C	N	O	0	0
			110	62	4	44		
3	D	9	Total	C	N	O	0	0
			110	62	4	44		
3	I	9	Total	C	N	O	0	0
			110	62	4	44		
3	J	9	Total	C	N	O	0	0
			110	62	4	44		
3	M	9	Total	C	N	O	0	0
			110	62	4	44		
3	N	9	Total	C	N	O	0	0
			110	62	4	44		

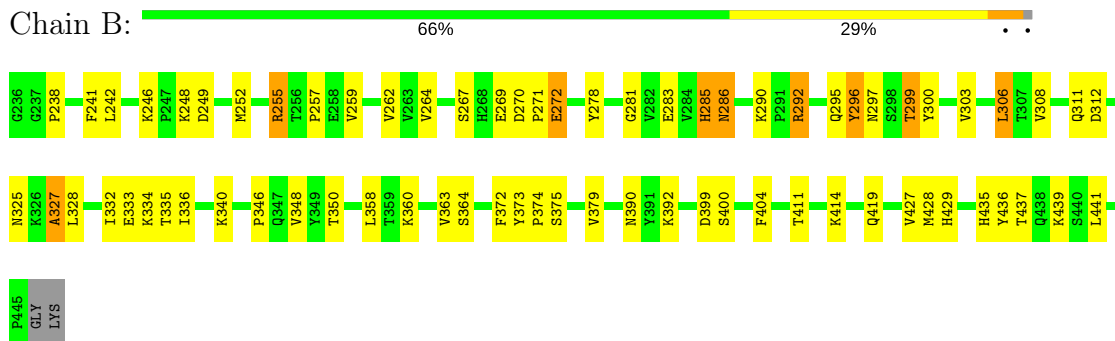
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

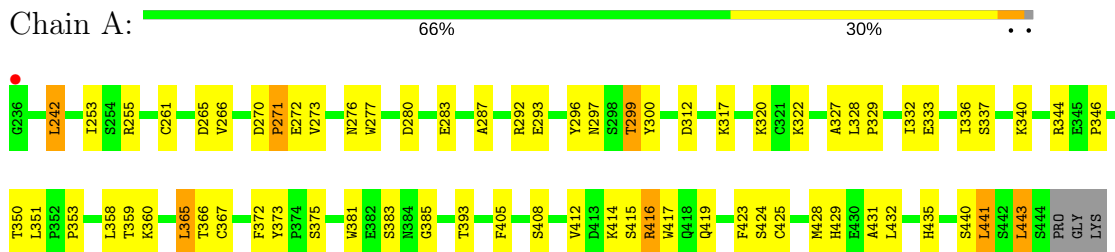
- Molecule 1: Ig gamma-1 chain C region



- Molecule 1: Ig gamma-1 chain C region

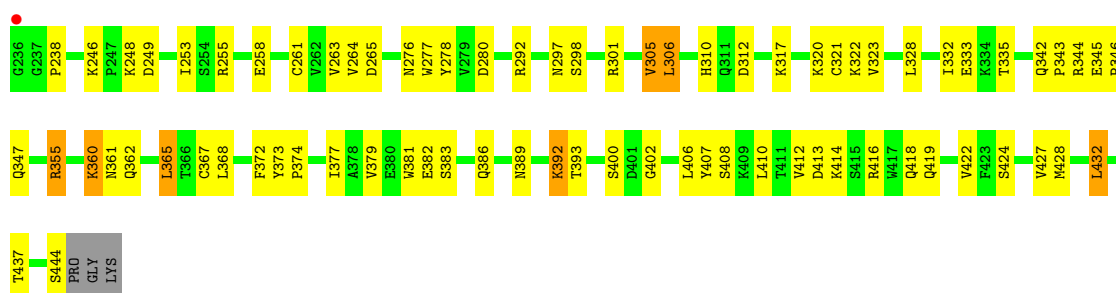


- Molecule 1: Ig gamma-1 chain C region

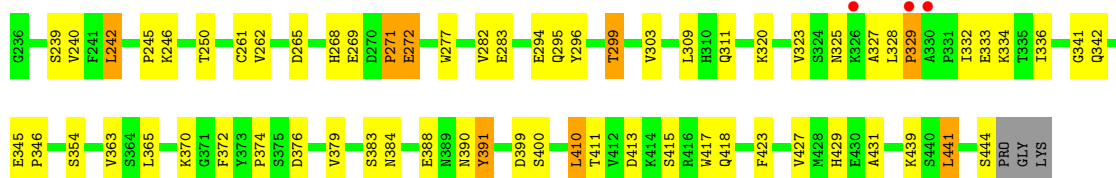


- Molecule 1: Ig gamma-1 chain C region

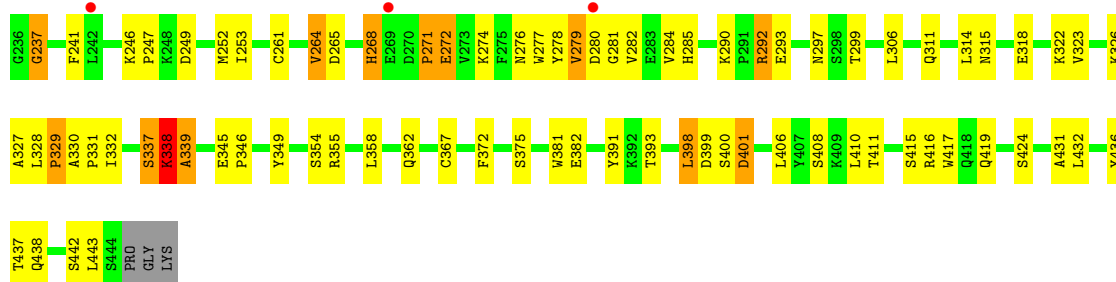




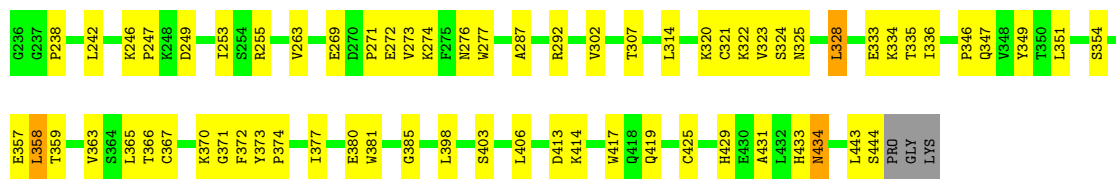
- Molecule 1: Ig gamma-1 chain C region



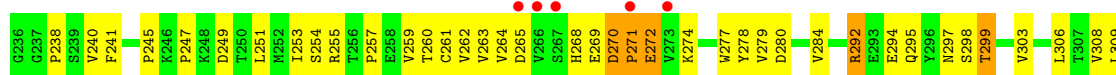
- Molecule 1: Ig gamma-1 chain C region

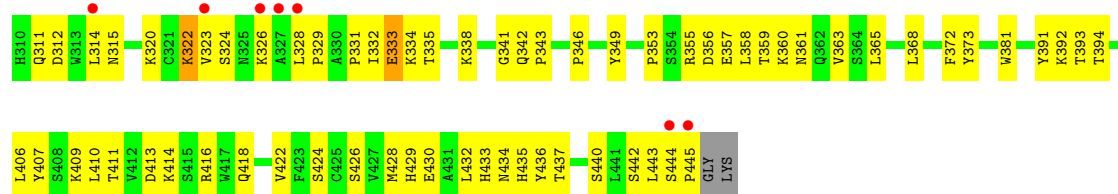


- Molecule 1: Ig gamma-1 chain C region

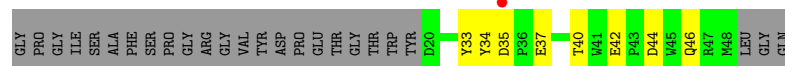
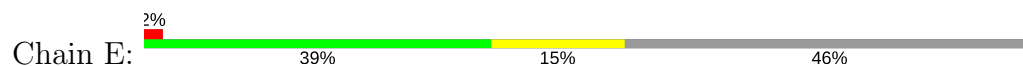


- Molecule 1: Ig gamma-1 chain C region

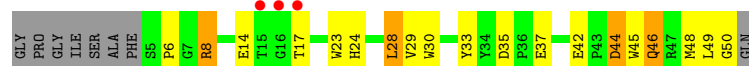




- Molecule 2: AFFinger p17



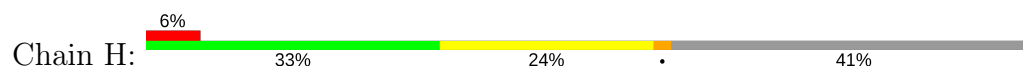
- Molecule 2: AFFinger p17



- Molecule 2: AFFinger p17



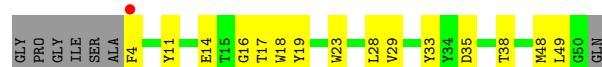
- Molecule 2: AFFinger p17



- Molecule 2: AFFinger p17

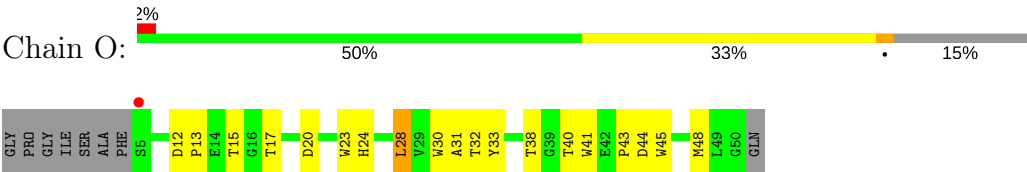


- Molecule 2: AFFinger p17

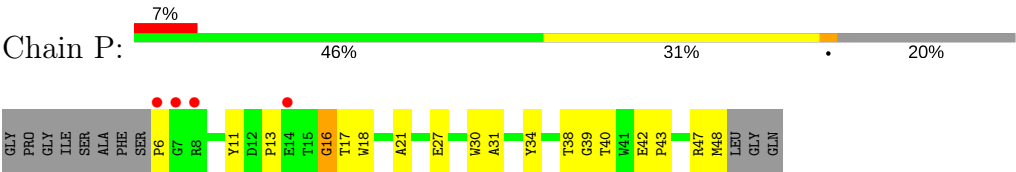


- Molecule 2: AFFinger p17





● Molecule 2: AFFinger p17



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.03Å 153.43Å 170.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 99.7 (49.74-2.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.200 , 0.242 0.200 , 0.243	Depositor DCC
$R_{free}$ test set	3079 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, GAL, NAG, BMA, 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	A	1.02	1/1714 (0.1%)	0.91	1/2335 (0.0%)
1	B	1.06	4/1722 (0.2%)	0.95	2/2347 (0.1%)
1	C	1.09	3/1714 (0.2%)	0.93	0/2335
1	D	0.98	2/1714 (0.1%)	0.89	0/2335
1	I	1.07	2/1714 (0.1%)	0.93	1/2335 (0.0%)
1	J	1.03	1/1714 (0.1%)	0.96	4/2335 (0.2%)
1	M	1.23	3/1714 (0.2%)	0.92	1/2335 (0.0%)
1	N	0.89	0/1722	0.84	0/2347
2	E	0.88	0/262	0.77	0/362
2	F	1.06	1/399 (0.3%)	0.82	0/551
2	G	1.01	0/411	0.79	0/567
2	H	0.91	0/287	0.74	0/396
2	K	0.98	0/399	0.88	1/551 (0.2%)
2	L	1.10	1/411 (0.2%)	0.84	0/567
2	O	0.90	0/399	0.84	0/551
2	P	0.91	0/381	0.75	0/526
All	All	1.04	18/16677 (0.1%)	0.90	10/22775 (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	I	0	1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	269	GLU	CD-OE1	24.76	1.52	1.25
1	M	269	GLU	CD-OE2	18.98	1.46	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	269	GLU	CD-OE1	16.57	1.43	1.25
1	D	360	LYS	CE-NZ	10.33	1.74	1.49
1	B	360	LYS	CE-NZ	9.37	1.72	1.49

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	PRO	C-N-CA	-11.56	92.80	121.70
1	B	271	PRO	CA-C-N	-8.15	99.28	117.20
1	A	265	ASP	CB-CG-OD1	7.08	124.67	118.30
1	J	249	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	K	47	ARG	NE-CZ-NH2	-6.47	117.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	296	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	1668	0	1633	45	1
1	B	1675	0	1640	55	0
1	C	1668	0	1633	48	1
1	D	1668	0	1633	55	0
1	I	1668	0	1633	46	0
1	J	1668	0	1633	54	0
1	M	1668	0	1633	46	0
1	N	1675	0	1639	90	0
2	E	250	0	211	4	0
2	F	381	0	327	8	0
2	G	392	0	336	10	0
2	H	274	0	234	10	0
2	K	381	0	327	8	0
2	L	392	0	336	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	381	0	327	17	0
2	P	363	0	309	16	0
3	A	110	0	94	0	0
3	B	110	0	94	6	0
3	C	110	0	94	0	0
3	D	110	0	94	4	0
3	I	110	0	94	2	0
3	J	110	0	94	5	0
3	M	110	0	94	4	0
3	N	110	0	94	10	0
All	All	17052	0	16236	507	1

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 507 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:D:501:NAG:H61	3:D:502:NAG:H82	1.19	1.07
1:I:390:ASN:HD22	1:I:411:THR:HB	1.19	1.07
2:O:30:TRP:HA	2:O:48:MET:HE1	1.33	1.07
1:M:246:LYS:HD2	1:M:247:PRO:HD2	1.31	1.05
1:I:242:LEU:HD13	1:I:336:ILE:HG12	1.32	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:NH2	1:A:287:ALA:O[2_454]	2.05	0.15

## 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	207/212 (98%)	192 (93%)	12 (6%)	3 (1%)	13	41
1	B	208/212 (98%)	191 (92%)	14 (7%)	3 (1%)	13	41
1	C	207/212 (98%)	196 (95%)	10 (5%)	1 (0%)	32	68
1	D	207/212 (98%)	200 (97%)	7 (3%)	0	100	100
1	I	207/212 (98%)	191 (92%)	13 (6%)	3 (1%)	13	41
1	J	207/212 (98%)	181 (87%)	17 (8%)	9 (4%)	3	12
1	M	207/212 (98%)	196 (95%)	9 (4%)	2 (1%)	18	51
1	N	208/212 (98%)	181 (87%)	23 (11%)	4 (2%)	9	33
2	E	27/54 (50%)	25 (93%)	1 (4%)	1 (4%)	4	16
2	F	44/54 (82%)	34 (77%)	6 (14%)	4 (9%)	1	2
2	G	45/54 (83%)	42 (93%)	3 (7%)	0	100	100
2	H	30/54 (56%)	22 (73%)	7 (23%)	1 (3%)	4	18
2	K	44/54 (82%)	40 (91%)	3 (7%)	1 (2%)	7	27
2	L	45/54 (83%)	41 (91%)	4 (9%)	0	100	100
2	O	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
2	P	41/54 (76%)	33 (80%)	6 (15%)	2 (5%)	2	9
All	All	1978/2128 (93%)	1804 (91%)	140 (7%)	34 (2%)	11	36

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	ALA
2	E	37	GLU
1	J	279	VAL
1	J	329	PRO
1	J	338	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	194/196 (99%)	182 (94%)	12 (6%)	21	52
1	B	195/196 (100%)	181 (93%)	14 (7%)	17	43
1	C	194/196 (99%)	185 (95%)	9 (5%)	31	65
1	D	194/196 (99%)	180 (93%)	14 (7%)	17	43
1	I	194/196 (99%)	177 (91%)	17 (9%)	12	34
1	J	194/196 (99%)	180 (93%)	14 (7%)	17	43
1	M	194/196 (99%)	186 (96%)	8 (4%)	35	70
1	N	195/196 (100%)	179 (92%)	16 (8%)	13	37
2	E	24/42 (57%)	21 (88%)	3 (12%)	5	16
2	F	37/42 (88%)	30 (81%)	7 (19%)	2	5
2	G	38/42 (90%)	35 (92%)	3 (8%)	14	39
2	H	26/42 (62%)	24 (92%)	2 (8%)	15	40
2	K	37/42 (88%)	34 (92%)	3 (8%)	14	38
2	L	38/42 (90%)	37 (97%)	1 (3%)	51	83
2	O	37/42 (88%)	36 (97%)	1 (3%)	50	82
2	P	35/42 (83%)	33 (94%)	2 (6%)	24	56
All	All	1826/1904 (96%)	1700 (93%)	126 (7%)	18	46

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	419	GLN
1	I	363	VAL
1	N	333	GLU
1	D	444	SER
2	H	37	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	325	ASN
1	I	295	GLN
1	M	429	HIS
1	D	389	ASN
1	D	419	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 ⓘ

72 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$
3	NAG	A	501	1,3	14,14,15	0.81	0	15,19,21	1.64	1 (6%)
3	NAG	A	502	3	14,14,15	0.70	0	15,19,21	1.42	2 (13%)
3	BMA	A	503	3	11,11,12	0.48	0	13,15,17	1.75	2 (15%)
3	MAN	A	504	3	11,11,12	0.71	0	13,15,17	2.32	6 (46%)
3	NAG	A	505	3	14,14,15	0.94	0	15,19,21	1.64	3 (20%)
3	MAN	A	506	3	11,11,12	0.70	0	13,15,17	0.99	0
3	GAL	A	507	3	11,11,12	1.25	1 (9%)	13,15,17	2.05	4 (30%)
3	FUC	A	508	3	9,10,11	1.11	0	13,14,16	1.59	3 (23%)
3	NAG	A	509	3	14,14,15	0.75	0	15,19,21	1.41	4 (26%)
3	NAG	B	501	1,3	14,14,15	0.98	1 (7%)	15,19,21	1.51	4 (26%)
3	NAG	B	502	3	14,14,15	0.70	0	15,19,21	1.54	3 (20%)
3	BMA	B	503	3	11,11,12	0.89	1 (9%)	13,15,17	1.71	2 (15%)
3	MAN	B	504	3	11,11,12	0.55	0	13,15,17	1.42	2 (15%)
3	NAG	B	505	3	14,14,15	0.60	0	15,19,21	1.83	3 (20%)
3	MAN	B	506	3	11,11,12	0.69	0	13,15,17	0.96	0
3	GAL	B	507	3	11,11,12	1.05	1 (9%)	13,15,17	1.78	4 (30%)
3	FUC	B	508	3	9,10,11	1.00	0	13,14,16	1.12	2 (15%)
3	NAG	B	509	3	14,14,15	0.63	0	15,19,21	1.72	3 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	501	1,3	14,14,15	0.65	0	15,19,21	1.47	3 (20%)
3	NAG	C	502	3	14,14,15	0.64	0	15,19,21	1.18	1 (6%)
3	BMA	C	503	3	11,11,12	0.74	0	13,15,17	1.02	1 (7%)
3	MAN	C	504	3	11,11,12	0.71	0	13,15,17	1.69	3 (23%)
3	NAG	C	505	3	14,14,15	0.53	0	15,19,21	1.24	1 (6%)
3	MAN	C	506	3	11,11,12	0.78	0	13,15,17	1.93	3 (23%)
3	GAL	C	507	3	11,11,12	0.95	0	13,15,17	2.52	4 (30%)
3	FUC	C	508	3	9,10,11	0.90	0	13,14,16	1.40	2 (15%)
3	NAG	C	509	3	14,14,15	0.48	0	15,19,21	2.21	3 (20%)
3	NAG	D	501	1,3	14,14,15	0.86	0	15,19,21	1.52	3 (20%)
3	NAG	D	502	3	14,14,15	0.74	0	15,19,21	1.83	4 (26%)
3	BMA	D	503	3	11,11,12	1.27	1 (9%)	13,15,17	1.54	3 (23%)
3	MAN	D	504	3	11,11,12	0.82	0	13,15,17	1.83	4 (30%)
3	NAG	D	505	3	14,14,15	0.73	0	15,19,21	1.52	4 (26%)
3	MAN	D	506	3	11,11,12	0.74	0	13,15,17	1.09	1 (7%)
3	GAL	D	507	3	11,11,12	0.70	0	13,15,17	1.87	4 (30%)
3	FUC	D	508	3	9,10,11	0.93	0	13,14,16	0.93	0
3	NAG	D	509	3	14,14,15	0.71	0	15,19,21	1.54	2 (13%)
3	NAG	I	501	1,3	14,14,15	0.75	0	15,19,21	1.66	3 (20%)
3	NAG	I	502	3	14,14,15	0.80	0	15,19,21	1.64	3 (20%)
3	BMA	I	503	3	11,11,12	0.76	0	13,15,17	0.99	1 (7%)
3	MAN	I	504	3	11,11,12	0.70	0	13,15,17	1.61	4 (30%)
3	NAG	I	505	3	14,14,15	0.73	0	15,19,21	1.51	2 (13%)
3	MAN	I	506	3	11,11,12	0.73	0	13,15,17	1.33	2 (15%)
3	GAL	I	507	3	11,11,12	1.01	1 (9%)	13,15,17	1.31	1 (7%)
3	FUC	I	508	3	9,10,11	0.82	0	13,14,16	0.99	1 (7%)
3	NAG	I	509	3	14,14,15	0.60	0	15,19,21	1.08	1 (6%)
3	NAG	J	501	1,3	14,14,15	0.84	0	15,19,21	1.47	3 (20%)
3	NAG	J	502	3	14,14,15	0.68	0	15,19,21	2.11	4 (26%)
3	BMA	J	503	3	11,11,12	0.59	0	13,15,17	1.18	1 (7%)
3	MAN	J	504	3	11,11,12	0.78	0	13,15,17	1.74	4 (30%)
3	NAG	J	505	3	14,14,15	0.67	0	15,19,21	1.67	3 (20%)
3	MAN	J	506	3	11,11,12	0.71	0	13,15,17	0.87	0
3	GAL	J	507	3	11,11,12	0.95	1 (9%)	13,15,17	1.57	3 (23%)
3	FUC	J	508	3	9,10,11	1.06	0	13,14,16	1.60	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	J	509	3	14,14,15	0.60	0	15,19,21	1.12	2 (13%)
3	NAG	M	501	1,3	14,14,15	0.54	0	15,19,21	1.32	3 (20%)
3	NAG	M	502	3	14,14,15	0.52	0	15,19,21	1.55	2 (13%)
3	BMA	M	503	3	11,11,12	0.69	0	13,15,17	1.57	1 (7%)
3	MAN	M	504	3	11,11,12	0.96	0	13,15,17	2.62	7 (53%)
3	NAG	M	505	3	14,14,15	0.95	0	15,19,21	1.52	2 (13%)
3	MAN	M	506	3	11,11,12	0.63	0	13,15,17	1.36	1 (7%)
3	GAL	M	507	3	11,11,12	1.01	1 (9%)	13,15,17	1.61	2 (15%)
3	FUC	M	508	3	9,10,11	1.04	0	13,14,16	1.77	5 (38%)
3	NAG	M	509	3	14,14,15	0.80	0	15,19,21	2.02	3 (20%)
3	NAG	N	501	1,3	14,14,15	0.53	0	15,19,21	1.33	1 (6%)
3	NAG	N	502	3	14,14,15	0.71	0	15,19,21	1.35	3 (20%)
3	BMA	N	503	3	11,11,12	0.66	0	13,15,17	0.70	0
3	MAN	N	504	3	11,11,12	0.71	0	13,15,17	1.61	2 (15%)
3	NAG	N	505	3	14,14,15	0.93	1 (7%)	15,19,21	1.33	4 (26%)
3	MAN	N	506	3	11,11,12	0.74	0	13,15,17	1.43	3 (23%)
3	GAL	N	507	3	11,11,12	1.06	1 (9%)	13,15,17	1.67	5 (38%)
3	FUC	N	508	3	9,10,11	0.82	0	13,14,16	0.99	1 (7%)
3	NAG	N	509	3	14,14,15	0.50	0	15,19,21	0.93	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
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3	-	0/6/23/26	0/1/1/1
3	BMA	A	503	3	-	0/2/19/22	0/1/1/1
3	MAN	A	504	3	-	0/2/19/22	0/1/1/1
3	NAG	A	505	3	-	0/6/23/26	0/1/1/1
3	MAN	A	506	3	-	0/2/19/22	0/1/1/1
3	GAL	A	507	3	-	0/2/19/22	0/1/1/1
3	FUC	A	508	3	-	0/0/17/20	0/1/1/1
3	NAG	A	509	3	-	1/6/23/26	0/1/1/1
3	NAG	B	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	502	3	-	0/6/23/26	0/1/1/1
3	BMA	B	503	3	-	0/2/19/22	0/1/1/1
3	MAN	B	504	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	505	3	-	0/6/23/26	0/1/1/1
3	MAN	B	506	3	-	0/2/19/22	0/1/1/1
3	GAL	B	507	3	-	0/2/19/22	0/1/1/1
3	FUC	B	508	3	-	0/0/17/20	0/1/1/1
3	NAG	B	509	3	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	502	3	-	0/6/23/26	0/1/1/1
3	BMA	C	503	3	-	0/2/19/22	0/1/1/1
3	MAN	C	504	3	-	0/2/19/22	0/1/1/1
3	NAG	C	505	3	-	0/6/23/26	0/1/1/1
3	MAN	C	506	3	-	0/2/19/22	0/1/1/1
3	GAL	C	507	3	-	0/2/19/22	0/1/1/1
3	FUC	C	508	3	-	0/0/17/20	0/1/1/1
3	NAG	C	509	3	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	502	3	-	0/6/23/26	0/1/1/1
3	BMA	D	503	3	-	0/2/19/22	0/1/1/1
3	MAN	D	504	3	-	0/2/19/22	0/1/1/1
3	NAG	D	505	3	-	0/6/23/26	0/1/1/1
3	MAN	D	506	3	-	0/2/19/22	0/1/1/1
3	GAL	D	507	3	-	0/2/19/22	0/1/1/1
3	FUC	D	508	3	-	0/0/17/20	0/1/1/1
3	NAG	D	509	3	-	0/6/23/26	0/1/1/1
3	NAG	I	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	502	3	-	0/6/23/26	0/1/1/1
3	BMA	I	503	3	-	0/2/19/22	0/1/1/1
3	MAN	I	504	3	-	0/2/19/22	0/1/1/1
3	NAG	I	505	3	-	0/6/23/26	0/1/1/1
3	MAN	I	506	3	-	0/2/19/22	0/1/1/1
3	GAL	I	507	3	-	0/2/19/22	0/1/1/1
3	FUC	I	508	3	-	0/0/17/20	0/1/1/1
3	NAG	I	509	3	-	0/6/23/26	0/1/1/1
3	NAG	J	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	502	3	-	0/6/23/26	0/1/1/1
3	BMA	J	503	3	-	0/2/19/22	0/1/1/1
3	MAN	J	504	3	-	0/2/19/22	0/1/1/1
3	NAG	J	505	3	-	0/6/23/26	0/1/1/1
3	MAN	J	506	3	-	0/2/19/22	0/1/1/1
3	GAL	J	507	3	-	0/2/19/22	0/1/1/1
3	FUC	J	508	3	-	0/0/17/20	0/1/1/1
3	NAG	J	509	3	-	1/6/23/26	0/1/1/1
3	NAG	M	501	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	502	3	-	0/6/23/26	0/1/1/1
3	BMA	M	503	3	-	0/2/19/22	0/1/1/1
3	MAN	M	504	3	-	0/2/19/22	0/1/1/1
3	NAG	M	505	3	-	0/6/23/26	0/1/1/1
3	MAN	M	506	3	-	0/2/19/22	0/1/1/1
3	GAL	M	507	3	-	0/2/19/22	0/1/1/1
3	FUC	M	508	3	-	0/0/17/20	0/1/1/1
3	NAG	M	509	3	-	0/6/23/26	0/1/1/1
3	NAG	N	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	502	3	-	0/6/23/26	0/1/1/1
3	BMA	N	503	3	-	0/2/19/22	0/1/1/1
3	MAN	N	504	3	-	0/2/19/22	0/1/1/1
3	NAG	N	505	3	-	0/6/23/26	0/1/1/1
3	MAN	N	506	3	-	0/2/19/22	0/1/1/1
3	GAL	N	507	3	-	0/2/19/22	0/1/1/1
3	FUC	N	508	3	-	0/0/17/20	0/1/1/1
3	NAG	N	509	3	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	503	BMA	C2-C3	-2.63	1.49	1.52
3	N	505	NAG	O5-C1	-2.23	1.40	1.43
3	B	503	BMA	C2-C3	2.02	1.55	1.52
3	I	507	GAL	C2-C3	2.17	1.55	1.52
3	N	507	GAL	C4-C5	2.18	1.57	1.53

The worst 5 of 181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	504	MAN	C1-O5-C5	-6.09	103.77	112.17
3	J	502	NAG	C2-N2-C7	-5.46	114.98	122.94
3	A	501	NAG	O5-C1-C2	-5.04	104.45	111.47
3	J	505	NAG	C1-O5-C5	-4.92	105.38	112.17
3	C	509	NAG	C3-C4-C5	-4.07	103.04	110.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	509	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	509	NAG	O7-C7-N2-C2

There are no ring outliers.

20 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	NAG	1	0
3	B	503	BMA	3	0
3	B	506	MAN	1	0
3	B	507	GAL	2	0
3	D	501	NAG	2	0
3	D	502	NAG	4	0
3	I	501	NAG	1	0
3	I	507	GAL	1	0
3	J	501	NAG	3	0
3	J	502	NAG	2	0
3	M	501	NAG	1	0
3	M	505	NAG	1	0
3	M	507	GAL	1	0
3	M	508	FUC	1	0
3	M	509	NAG	2	0
3	N	501	NAG	3	0
3	N	502	NAG	4	0
3	N	505	NAG	1	0
3	N	508	FUC	2	0
3	N	509	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	209/212 (98%)	-0.42	1 (0%) 90 90	20, 39, 61, 69	7 (3%)
1	B	210/212 (99%)	-0.32	0 100 100	21, 40, 72, 77	7 (3%)
1	C	209/212 (98%)	-0.39	0 100 100	16, 39, 68, 74	7 (3%)
1	D	209/212 (98%)	-0.36	1 (0%) 90 90	24, 43, 57, 67	7 (3%)
1	I	209/212 (98%)	-0.30	3 (1%) 75 74	20, 40, 68, 79	7 (3%)
1	J	209/212 (98%)	-0.18	3 (1%) 75 74	22, 45, 86, 94	4 (1%)
1	M	209/212 (98%)	-0.39	0 100 100	25, 44, 60, 64	7 (3%)
1	N	210/212 (99%)	0.08	12 (5%) 24 19	27, 58, 105, 108	7 (3%)
2	E	29/54 (53%)	0.22	1 (3%) 46 39	36, 64, 96, 101	0
2	F	46/54 (85%)	0.25	3 (6%) 20 15	36, 62, 98, 101	0
2	G	47/54 (87%)	0.21	4 (8%) 11 8	28, 50, 88, 100	0
2	H	32/54 (59%)	0.79	3 (9%) 9 6	55, 82, 98, 102	0
2	K	46/54 (85%)	-0.02	1 (2%) 62 59	25, 47, 80, 82	0
2	L	47/54 (87%)	-0.18	1 (2%) 64 60	31, 47, 74, 87	0
2	O	46/54 (85%)	-0.16	1 (2%) 62 59	44, 53, 74, 84	0
2	P	43/54 (79%)	0.48	4 (9%) 9 6	43, 75, 108, 114	0
All	All	2010/2128 (94%)	-0.21	38 (1%) 67 64	16, 45, 88, 114	53 (2%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLY	4.7
2	F	17	THR	4.2
2	F	15	THR	4.1
1	I	330	ALA	3.8
1	N	445	PRO	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
3	GAL	B	507	11/12	0.86	0.32	6.10	80,86,88,88	0
3	GAL	M	507	11/12	0.88	0.30	5.03	75,79,81,82	0
3	GAL	A	507	11/12	0.89	0.28	4.92	53,58,62,63	0
3	GAL	J	507	11/12	0.89	0.30	4.30	88,92,93,93	0
3	GAL	I	507	11/12	0.91	0.22	3.51	50,57,59,61	0
3	GAL	N	507	11/12	0.89	0.28	2.05	74,79,81,82	0
3	GAL	C	507	11/12	0.91	0.19	0.63	66,69,72,72	0
3	FUC	B	508	10/11	0.81	0.23	0.23	94,97,99,102	0
3	FUC	C	508	10/11	0.92	0.22	0.04	80,84,88,90	0
3	NAG	A	502	14/15	0.96	0.14	-0.52	47,51,53,54	0
3	NAG	A	505	14/15	0.96	0.14	-0.53	40,44,48,51	0
3	GAL	D	507	11/12	0.93	0.14	-0.60	66,70,72,75	0
3	NAG	B	501	14/15	0.91	0.15	-0.83	68,72,77,81	0
3	NAG	D	505	14/15	0.97	0.13	-0.93	47,51,53,53	0
3	NAG	I	505	14/15	0.95	0.14	-1.16	47,51,52,54	0
3	NAG	D	502	14/15	0.96	0.14	-1.18	42,46,51,54	0
3	NAG	C	502	14/15	0.96	0.12	-1.28	56,63,65,67	0
3	NAG	N	505	14/15	0.97	0.12	-1.52	68,69,74,74	0
3	NAG	C	505	14/15	0.93	0.13	-1.95	64,74,79,80	0
3	NAG	J	502	14/15	0.93	0.16	-2.48	62,70,74,74	0
3	BMA	I	503	11/12	0.95	0.12	-	62,63,64,68	0
3	NAG	D	509	14/15	0.84	0.18	-	72,81,86,89	0
3	NAG	B	509	14/15	0.75	0.21	-	103,108,110,111	0
3	FUC	D	508	10/11	0.90	0.14	-	79,85,86,86	0
3	MAN	M	506	11/12	0.91	0.14	-	78,83,84,90	0
3	NAG	N	509	14/15	0.88	0.14	-	106,108,109,110	0
3	NAG	B	505	14/15	0.93	0.18	-	78,81,91,94	0
3	BMA	A	503	11/12	0.97	0.10	-	50,53,53,58	0
3	MAN	C	504	11/12	0.91	0.17	-	74,77,84,86	0
3	BMA	M	503	11/12	0.95	0.11	-	53,57,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	I	502	14/15	0.95	0.16	-	52,60,62,62	0
3	FUC	J	508	10/11	0.90	0.24	-	86,89,91,92	0
3	BMA	D	503	11/12	0.96	0.11	-	45,46,48,52	0
3	NAG	M	502	14/15	0.98	0.12	-	52,56,57,58	0
3	MAN	B	506	11/12	0.92	0.14	-	84,86,88,95	0
3	FUC	N	508	10/11	0.83	0.31	-	103,106,108,108	0
3	MAN	D	506	11/12	0.96	0.12	-	55,57,58,66	0
3	MAN	J	506	11/12	0.89	0.18	-	97,101,104,107	0
3	NAG	J	505	14/15	0.94	0.13	-	60,62,64,72	0
3	NAG	I	501	14/15	0.93	0.17	-	64,66,70,70	0
3	FUC	M	508	10/11	0.94	0.17	-	77,79,82,82	0
3	NAG	D	501	14/15	0.95	0.19	-	49,52,58,65	0
3	BMA	B	503	11/12	0.94	0.11	-	71,74,77,78	0
3	NAG	A	501	14/15	0.93	0.14	-	54,58,68,69	0
3	NAG	M	501	14/15	0.97	0.12	-	57,59,62,68	0
3	BMA	C	503	11/12	0.93	0.12	-	68,71,74,79	0
3	MAN	J	504	11/12	0.97	0.12	-	65,68,69,70	0
3	NAG	C	509	14/15	0.87	0.19	-	97,100,102,105	0
3	MAN	C	506	11/12	0.92	0.15	-	90,92,93,95	0
3	NAG	I	509	14/15	0.91	0.18	-	89,94,95,95	0
3	NAG	N	502	14/15	0.90	0.14	-	83,89,91,92	0
3	MAN	I	506	11/12	0.92	0.12	-	71,74,77,83	0
3	BMA	J	503	11/12	0.87	0.12	-	72,82,85,92	0
3	NAG	M	505	14/15	0.96	0.13	-	42,53,57,61	0
3	MAN	N	506	11/12	0.85	0.14	-	97,100,101,104	0
3	NAG	J	501	14/15	0.94	0.11	-	66,69,72,77	0
3	NAG	M	509	14/15	0.73	0.31	-	102,106,108,108	0
3	FUC	I	508	10/11	0.93	0.21	-	75,79,81,83	0
3	MAN	A	504	11/12	0.94	0.16	-	48,54,55,56	0
3	MAN	B	504	11/12	0.94	0.11	-	80,82,85,88	0
3	FUC	A	508	10/11	0.86	0.18	-	82,87,89,89	0
3	NAG	C	501	14/15	0.95	0.18	-	62,64,67,74	0
3	MAN	I	504	11/12	0.94	0.12	-	49,50,53,54	0
3	NAG	A	509	14/15	0.87	0.12	-	78,89,90,91	0
3	BMA	N	503	11/12	0.92	0.10	-	79,86,89,93	0
3	MAN	M	504	11/12	0.94	0.15	-	54,56,62,63	0
3	MAN	N	504	11/12	0.96	0.12	-	65,67,70,71	0
3	NAG	N	501	14/15	0.87	0.25	-	94,98,100,101	0
3	MAN	D	504	11/12	0.96	0.11	-	40,45,48,49	0
3	MAN	A	506	11/12	0.95	0.12	-	63,64,66,72	0
3	NAG	J	509	14/15	0.82	0.22	-	107,111,113,113	0
3	NAG	B	502	14/15	0.96	0.12	-	61,64,67,67	0



## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.