



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 02:51 PM GMT

PDB ID : 2J1G  
Title : L-ficolin complexed to N-acetyl-cystein  
Authors : Garlatti, V.; Gaboriaud, C.  
Deposited on : 2006-08-11  
Resolution : 1.95 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>

---

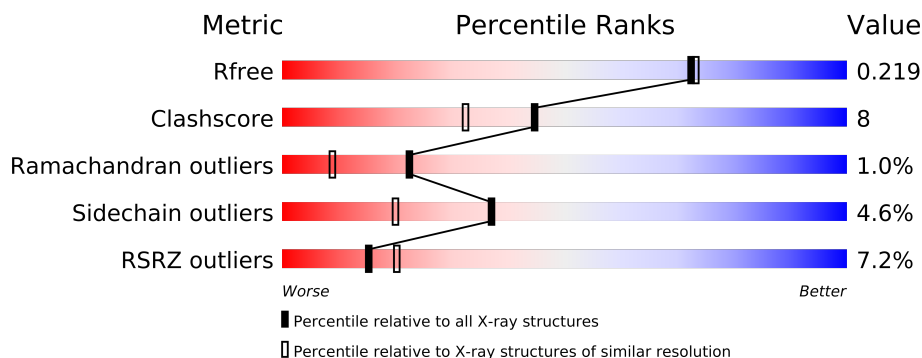
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	A	218	
1	B	218	
1	C	218	
1	D	218	
1	E	218	
1	F	218	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	B	1290	-	X
5	P4C	B	1297	X	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
5	P4C	E	1293	-	X
7	SC2	F	1290	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11289 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.

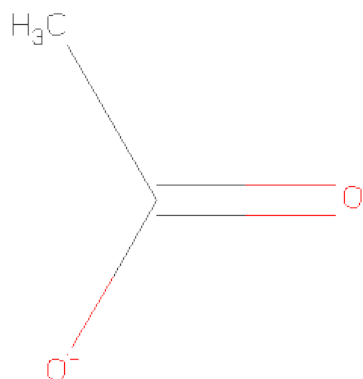
- Molecule 1 is a protein called FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	3	0
			1617	1025	280	305	7			
1	B	217	Total	C	N	O	S	0	0	0
			1736	1092	305	330	9			
1	C	216	Total	C	N	O	S	0	0	0
			1729	1087	304	329	9			
1	D	214	Total	C	N	O	S	0	0	0
			1715	1078	302	327	8			
1	E	218	Total	C	N	O	S	0	1	0
			1755	1102	311	333	9			
1	F	217	Total	C	N	O	S	0	0	0
			1736	1092	305	330	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	THR	VAL	CONFLICT	UNP Q15485
A	247	THR	VAL	CONFLICT	UNP Q15485
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485
C	168	THR	VAL	CONFLICT	UNP Q15485
C	247	THR	VAL	CONFLICT	UNP Q15485
D	168	THR	VAL	CONFLICT	UNP Q15485
D	247	THR	VAL	CONFLICT	UNP Q15485
E	168	THR	VAL	CONFLICT	UNP Q15485
E	247	THR	VAL	CONFLICT	UNP Q15485
F	168	THR	VAL	CONFLICT	UNP Q15485
F	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		

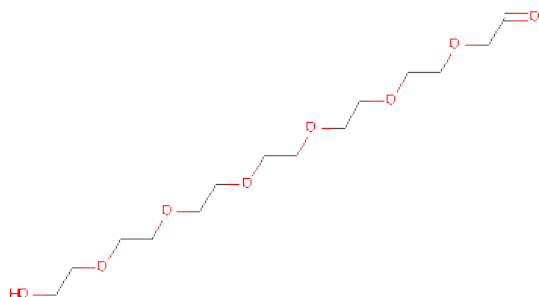
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			60	34	2	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	168	THR	VAL	CONFLICT	UNP Q15485
B	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 5 is O-ACETALDEHYDYL-HEXAETHYLENEGLYCOL (three-letter code: P4C) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	5	0
			18	12	6		
5	B	1	Total	C	O	4	0
			4	2	2		
5	E	1	Total	C	O	0	0
			17	11	6		
5	E	1	Total	C	O	5	0
			5	3	2		

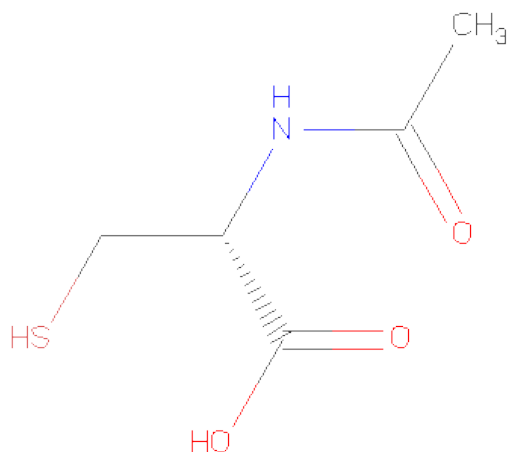
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	2	Total	C	N	O	0	0
			28	16	2	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	168	THR	VAL	CONFLICT	UNP Q15485
E	247	THR	VAL	CONFLICT	UNP Q15485

- Molecule 7 is N-ACETYL-L-CYSTEINE (three-letter code: SC2) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	N	O	S	2	0
			10	5	1	3	1		

- Molecule 8 is water.

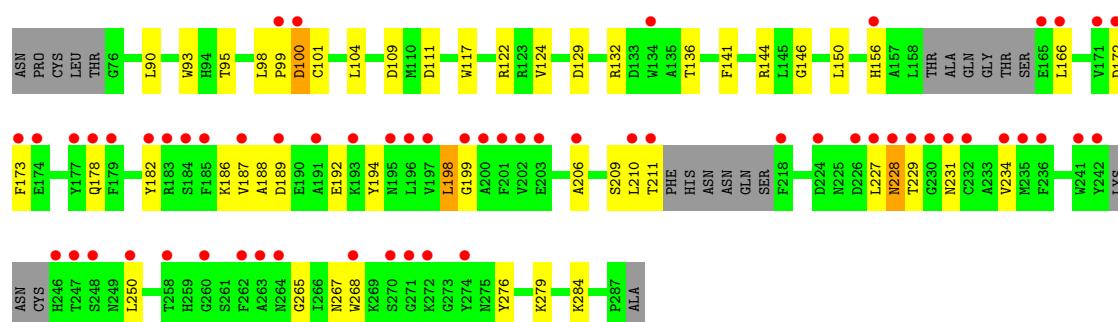
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	206	Total	O	0	0
			206	206		
8	C	169	Total	O	0	0
			169	169		
8	D	92	Total	O	0	0
			92	92		
8	E	190	Total	O	0	0
			190	190		
8	F	104	Total	O	0	0
			104	104		

### 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: FICOLIN-2

Chain A: 



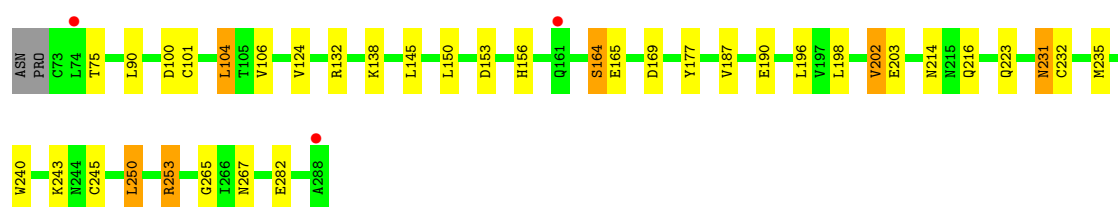
#### • Molecule 1: FICOLIN-2

Chain B: 



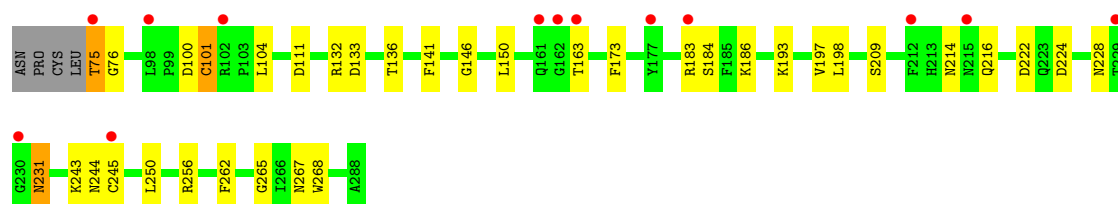
#### • Molecule 1: FICOLIN-2

Chain C: 



#### • Molecule 1: FICOLIN-2

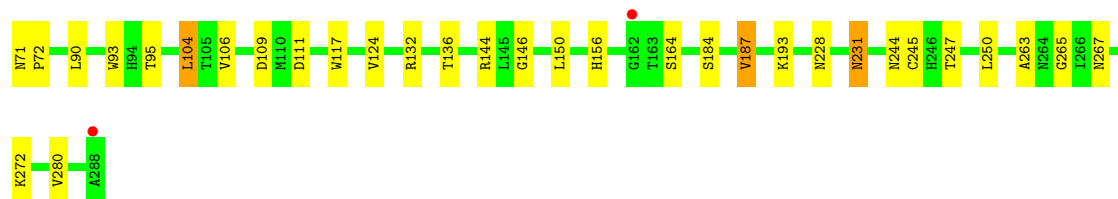
Chain D: 





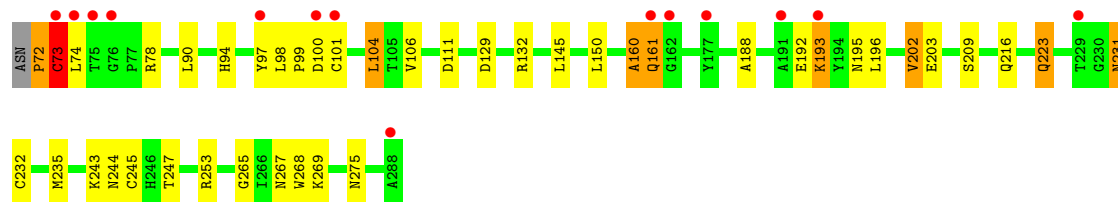
- Molecule 1: FICOLIN-2

Chain E:



- Molecule 1: FICOLIN-2

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.04Å 99.04Å 142.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 1.95 19.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.95) 99.9 (19.76-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176 , 0.210 0.189 , 0.219	Depositor DCC
$R_{free}$ test set	5667 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.9	EDS
Estimated twinning fraction	0.011 for -h,-k,l 0.049 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 113326 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, CA, P4C, FUC, ACT, SC2, 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	0.32	0/1660	0.47	0/2242
1	B	0.48	0/1784	0.59	0/2413
1	C	0.44	0/1776	0.64	1/2402 (0.0%)
1	D	0.35	0/1762	0.51	0/2383
1	E	0.44	0/1803	0.60	0/2439
1	F	0.87	4/1784 (0.2%)	0.97	7/2413 (0.3%)
All	All	0.52	4/10569 (0.0%)	0.65	8/14292 (0.1%)

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	F	1	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	72	PRO	N-CA	-27.40	1.00	1.47
1	F	73	CYS	CA-C	-13.04	1.19	1.52
1	F	72	PRO	CA-CB	11.09	1.75	1.53
1	F	73	CYS	CA-CB	-6.87	1.38	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	CYS	CB-CA-C	21.12	152.65	110.40
1	F	72	PRO	N-CA-C	17.55	157.72	112.10
1	F	72	PRO	CB-CA-C	-16.55	70.62	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	CYS	N-CA-CB	-14.63	84.27	110.60
1	F	73	CYS	CA-CB-SG	-10.22	95.61	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	73	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	73	CYS	Mainchain

## 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	A	1617	0	1493	29	0
1	B	1736	0	1608	20	0
1	C	1729	0	1603	26	0
1	D	1715	0	1585	25	0
1	E	1755	0	1623	23	0
1	F	1736	0	1609	47	0
2	B	4	0	3	0	0
2	C	8	0	6	4	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	B	60	0	52	1	0
5	B	22	0	26	0	0
5	E	22	0	24	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	28	0	25	0	0
7	F	10	0	8	1	0
8	A	73	0	0	4	0
8	B	206	0	0	4	0
8	C	169	0	0	7	0
8	D	92	0	0	4	0
8	E	190	0	0	3	0
8	F	104	0	0	9	0
All	All	11289	0	9671	168	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 8.

The worst 5 of 168 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:72:PRO:CB	1:F:72:PRO:CA	1.75	1.40
1:F:72:PRO:C	1:F:72:PRO:CB	1.90	1.36
1:F:72:PRO:CB	1:F:73:CYS:N	2.00	1.25
1:B:216:GLN:HE21	1:B:243:LYS:CE	1.53	1.22
1:B:216:GLN:NE2	1:B:243:LYS:HE3	1.57	1.19

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	192/218 (88%)	174 (91%)	13 (7%)	5 (3%)	8	1
1	B	215/218 (99%)	203 (94%)	11 (5%)	1 (0%)	38	23
1	C	214/218 (98%)	200 (94%)	13 (6%)	1 (0%)	38	23
1	D	212/218 (97%)	201 (95%)	10 (5%)	1 (0%)	38	23
1	E	217/218 (100%)	206 (95%)	9 (4%)	2 (1%)	25	11
1	F	215/218 (99%)	201 (94%)	12 (6%)	2 (1%)	25	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1265/1308 (97%)	1185 (94%)	68 (5%)	12 (1%)	22	11

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	ASN
1	F	73	CYS
1	F	160	ALA
1	A	229	THR
1	A	198	LEU

### 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	168/183 (92%)	161 (96%)	7 (4%)	40	24
1	B	182/183 (100%)	176 (97%)	6 (3%)	50	35
1	C	181/183 (99%)	171 (94%)	10 (6%)	30	14
1	D	179/183 (98%)	171 (96%)	8 (4%)	38	21
1	E	184/183 (100%)	176 (96%)	8 (4%)	40	23
1	F	182/183 (100%)	172 (94%)	10 (6%)	30	14
All	All	1076/1098 (98%)	1027 (95%)	49 (5%)	37	20

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	250	LEU
1	D	183	ARG
1	F	196	LEU
1	D	101	CYS
1	D	193	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	139	GLN
1	D	216	GLN
1	F	216	GLN
1	D	156	HIS
1	D	195	ASN

### 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 ⓘ

7 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	B	1291	1,4	12,14,15	0.67	0	15,19,21	1.33	3 (20%)
4	NAG	B	1292	4	12,14,15	0.69	0	15,19,21	0.95	1 (6%)
4	FUC	B	1293	4	9,10,11	0.71	0	10,14,16	1.05	0
4	BMA	B	1294	4	10,11,12	0.85	1 (10%)	11,15,17	1.37	2 (18%)
4	MAN	B	1295	4	10,11,12	0.75	0	11,15,17	1.24	2 (18%)
6	NAG	E	1291	1,6	12,14,15	0.68	1 (8%)	15,19,21	1.11	1 (6%)
6	NAG	E	1292	6	12,14,15	0.64	0	15,19,21	1.28	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
4	NAG	B	1291	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1292	4	-	0/6/23/26	0/1/1/1
4	FUC	B	1293	4	-	0/0/17/20	0/1/1/1
4	BMA	B	1294	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1295	4	-	0/2/19/22	0/1/1/1
6	NAG	E	1291	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	1292	6	-	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)
6	E	1291	NAG	O5-C5	-2.13	1.41	1.45
4	B	1294	BMA	O5-C5	-2.04	1.41	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1292	NAG	O5-C5-C6	4.00	111.18	106.98
6	E	1291	NAG	O5-C5-C6	2.86	109.98	106.98
4	B	1294	BMA	C4-C3-C2	2.74	114.19	110.50
4	B	1291	NAG	O5-C5-C6	2.61	109.72	106.98
4	B	1294	BMA	O5-C5-C6	2.54	109.65	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

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	ACT	B	1289	-	1,3,3	0.91	0	0,3,3	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	P4C	B	1296	1	17,17,21	4.89	3 (17%)	15,16,20	4.44	3 (20%)
5	P4C	B	1297	-	3,3,21	2.48	2 (66%)	2,2,20	3.09	1 (50%)
2	ACT	C	1289	-	1,3,3	1.30	0	0,3,3	0.00	-
2	ACT	C	1290	-	1,3,3	0.98	0	0,3,3	0.00	-
2	ACT	E	1289	-	1,3,3	1.38	0	0,3,3	0.00	-
5	P4C	E	1293	-	15,16,21	1.04	1 (6%)	14,15,20	0.45	0
5	P4C	E	1294	-	3,4,21	1.92	1 (33%)	2,3,20	3.86	2 (100%)
2	ACT	F	1289	-	1,3,3	0.97	0	0,3,3	0.00	-
7	SC2	F	1290	-	9,9,9	1.57	1 (11%)	11,11,11	2.95	2 (18%)

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	ACT	B	1289	-	-	0/0/0/0	0/0/0/0
5	P4C	B	1296	1	-	0/15/15/19	0/0/0/0
5	P4C	B	1297	-	-	0/1/1/19	0/0/0/0
2	ACT	C	1289	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1290	-	-	0/0/0/0	0/0/0/0
2	ACT	E	1289	-	-	0/0/0/0	0/0/0/0
5	P4C	E	1293	-	-	0/14/14/19	0/0/0/0
5	P4C	E	1294	-	-	0/2/2/19	0/0/0/0
2	ACT	F	1289	-	-	0/0/0/0	0/0/0/0
7	SC2	F	1290	-	-	0/10/10/10	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1296	P4C	C15-C14	-19.17	0.48	1.48
5	B	1296	P4C	C2-C3	-4.60	1.53	1.55
7	F	1290	SC2	OT-CT	-4.31	1.13	1.23
5	E	1293	P4C	O1-C2	-3.50	1.23	1.42
5	B	1296	P4C	O16-C17	3.49	1.57	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1296	P4C	O13-C14-C15	12.95	169.21	110.47
5	B	1296	P4C	O16-C15-C14	10.37	157.51	110.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1290	SC2	OT-CT-CM	-8.65	105.16	122.04
5	E	1294	P4C	O7-C6-C5	4.79	131.09	114.71
5	B	1297	P4C	O1-C2-C3	4.36	124.65	111.72

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	A	197/218 (90%)	1.62	60 (30%) 1 0	32, 51, 84, 95	1 (0%)
1	B	217/218 (99%)	0.01	1 (0%) 88 94	24, 28, 38, 49	0
1	C	216/218 (99%)	-0.06	3 (1%) 72 80	21, 28, 39, 60	2 (0%)
1	D	214/218 (98%)	0.44	13 (6%) 21 26	37, 43, 55, 63	0
1	E	218/218 (100%)	0.12	2 (0%) 81 88	28, 32, 40, 53	1 (0%)
1	F	217/218 (99%)	0.58	14 (6%) 18 24	29, 36, 47, 53	5 (2%)
All	All	1279/1308 (97%)	0.43	93 (7%) 15 19	21, 35, 59, 95	9 (0%)

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	10.3
1	F	74	LEU	8.2
1	F	75	THR	7.7
1	A	247	THR	7.1
1	A	230	GLY	6.8

### 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 ⓘ

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
6	NAG	E	1292	14/15	0.13	3.25	47,48,49,49	0
4	MAN	B	1295	11/12	0.16	3.11	46,48,49,50	0
4	FUC	B	1293	10/11	0.16	1.84	38,41,42,44	0
4	BMA	B	1294	11/12	0.11	0.89	44,47,48,48	0
6	NAG	E	1291	14/15	0.10	-0.05	42,46,47,48	0
4	NAG	B	1291	14/15	0.09	-0.09	27,28,33,38	0
4	NAG	B	1292	14/15	0.10	-0.62	33,34,39,41	0

## 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
7	SC2	F	1290	10/10	0.23	7.65	48,54,54,54	5
5	P4C	E	1293	17/22	0.23	3.93	54,58,66,67	0
3	CA	B	1290	1/1	0.11	3.67	25,25,25,25	0
2	ACT	C	1290	4/4	0.12	1.69	38,39,39,39	4
2	ACT	C	1289	4/4	0.10	0.62	30,30,31,32	0
3	CA	E	1290	1/1	0.11	0.53	25,25,25,25	0
2	ACT	E	1289	4/4	0.11	0.29	41,41,41,41	0
5	P4C	B	1296	18/22	0.13	0.19	20,45,48,48	5
3	CA	C	1291	1/1	0.08	-0.17	29,29,29,29	0
2	ACT	F	1289	4/4	0.10	-0.94	44,44,45,45	0
3	CA	D	1289	1/1	0.04	-2.01	53,53,53,53	0
2	ACT	B	1289	4/4	0.07	-2.21	38,39,39,40	0
3	CA	F	1291	1/1	0.11	-2.38	52,52,52,52	0
5	P4C	B	1297	4/22	-	-	72,74,74,74	4
5	P4C	E	1294	5/22	-	-	20,20,20,20	5

## 6.5 Other polymers ⓘ

There are no such residues in this entry.