



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID : 2Q7N  
Title : Crystal structure of Leukemia inhibitory factor in complex with LIF receptor (domains 1-5)  
Authors : Huyton, T.; Zhang, J.G.; Nicola, N.A.; Garrett, T.P.J.  
Deposited on : 2007-06-07  
Resolution : 4.00 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.

---

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

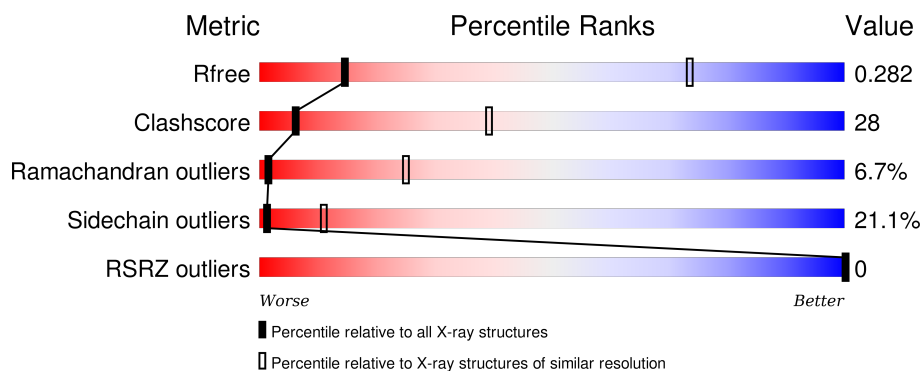
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	488	<div> <div>43%</div> <div>42%</div> <div>13%</div> <div>..</div> </div>
1	C	488	<div> <div>46%</div> <div>40%</div> <div>11%</div> <div>..</div> </div>
2	B	180	<div> <div>47%</div> <div>39%</div> <div>13%</div> <div>.</div> </div>
2	D	180	<div> <div>42%</div> <div>46%</div> <div>12%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	N	401	-	-	X	-
3	NAG	N	403	-	-	X	-
3	NAG	O	501	X	-	-	-
4	NAG	F	201	-	-	X	X
4	NAG	F	203	-	-	X	-
4	NAG	S	901	-	-	X	-
5	NAG	C	501	-	-	-	X
6	MAN	J	703	X	-	-	-
7	MAN	K	804	X	-	-	-
8	MAN	R	804	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10839 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 Leukemia inhibitory factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2369	642	711	17			
1	C	480	Total	C	N	O	S	0	0	0
			3739	2369	642	711	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	CLONING ARTIFACT	UNP P42703
A	0	TYR	-	CLONING ARTIFACT	UNP P42703
A	1	LYS	-	CLONING ARTIFACT	UNP P42703
A	2	ASP	-	CLONING ARTIFACT	UNP P42703
A	3	ASP	-	CLONING ARTIFACT	UNP P42703
A	4	ASP	-	CLONING ARTIFACT	UNP P42703
A	5	ASP	-	CLONING ARTIFACT	UNP P42703
A	6	LYS	-	CLONING ARTIFACT	UNP P42703
C	-1	ASP	-	CLONING ARTIFACT	UNP P42703
C	0	TYR	-	CLONING ARTIFACT	UNP P42703
C	1	LYS	-	CLONING ARTIFACT	UNP P42703
C	2	ASP	-	CLONING ARTIFACT	UNP P42703
C	3	ASP	-	CLONING ARTIFACT	UNP P42703
C	4	ASP	-	CLONING ARTIFACT	UNP P42703
C	5	ASP	-	CLONING ARTIFACT	UNP P42703
C	6	LYS	-	CLONING ARTIFACT	UNP P42703

- Molecule 2 is a protein called Leukemia inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1387	884	245	251	7			
2	D	180	Total	C	N	O	S	0	0	0
			1387	884	245	251	7			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	3	Total	C	N	O	0	0
			38	22	2	14		
3	H	3	Total	C	N	O	0	0
			38	22	2	14		
3	I	3	Total	C	N	O	0	0
			38	22	2	14		
3	N	3	Total	C	N	O	0	0
			38	22	2	14		
3	O	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	4	Total	C	N	O	0	0
			49	28	2	19		

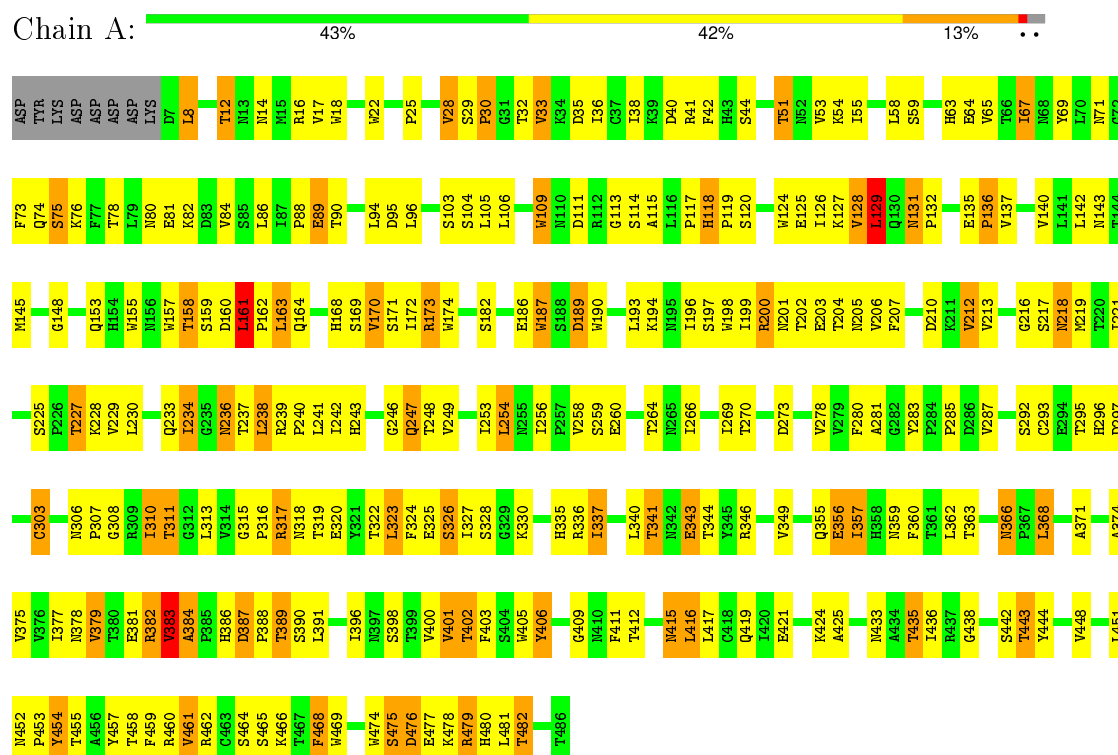
- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

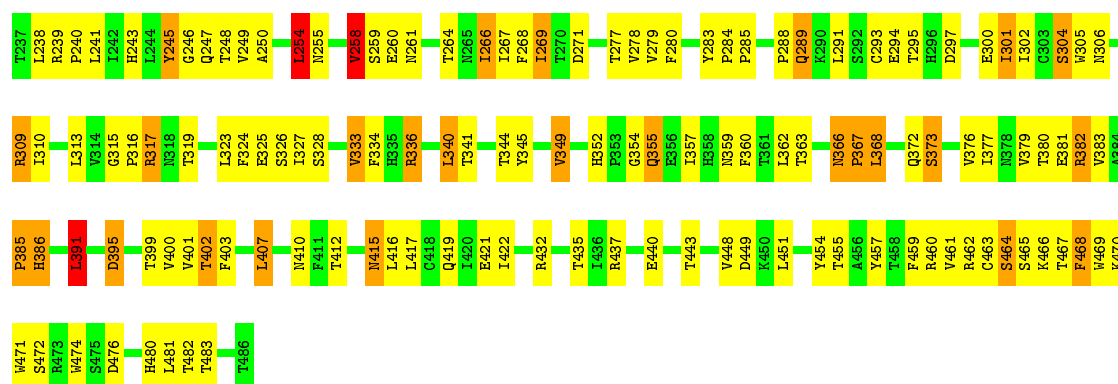
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	R	5	Total	C	N	O	0	0
			60	34	2	24		

### 3 Residue-property plots

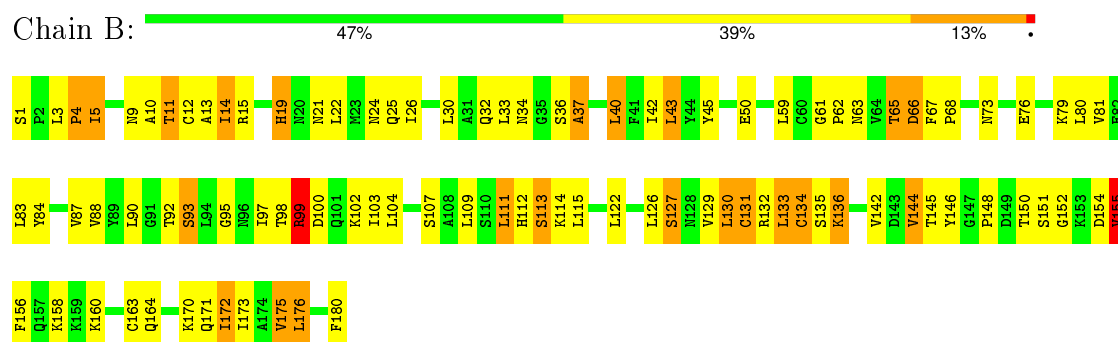
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

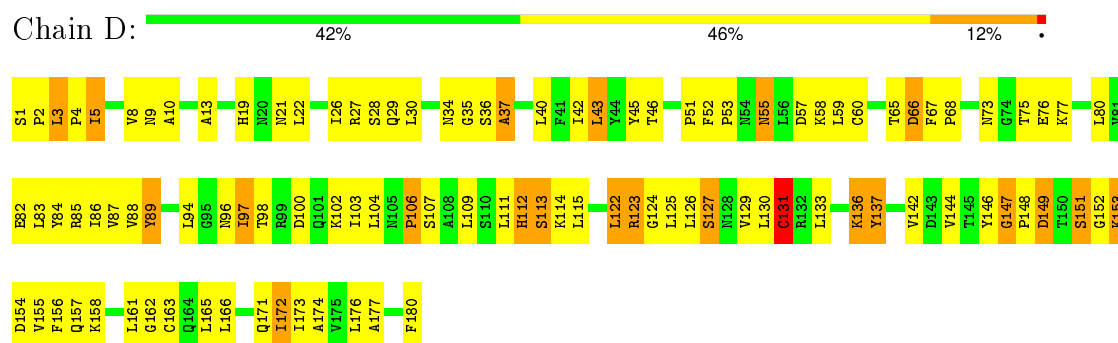




- Molecule 2: Leukemia inhibitory factor



- Molecule 2: Leukemia inhibitory factor





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.48Å 240.13Å 202.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 19.98 – 4.01	Depositor EDS
% Data completeness (in resolution range)	93.6 (20.00-4.00) 93.6 (19.98-4.01)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.237 , 0.287 0.232 , 0.282	Depositor DCC
$R_{free}$ test set	1852 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	119.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 81.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 37091 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	10839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.76	2/3842 (0.1%)	0.82	2/5267 (0.0%)
1	C	0.73	0/3842	0.82	2/5267 (0.0%)
2	B	0.73	0/1416	0.77	0/1923
2	D	0.73	0/1416	0.81	0/1923
All	All	0.74	2/10516 (0.0%)	0.81	4/14380 (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	C	0	2
3	O	1	0
6	J	1	0
7	K	1	0
8	R	1	0
All	All	4	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	VAL	CA-CB	5.65	1.66	1.54
1	A	303	CYS	CB-SG	-5.65	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	LEU	CA-CB-CG	7.97	133.63	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	254	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	391	LEU	CA-CB-CG	5.14	127.12	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	J	703	MAN	C1
7	K	804	MAN	C1
3	O	501	NAG	C1
8	R	804	MAN	C1

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ARG	Peptide
1	A	384	ALA	Peptide
1	C	28	VAL	Peptide
1	C	40	ASP	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	3739	0	3568	210	0
1	C	3739	0	3568	205	0
2	B	1387	0	1417	78	0
2	D	1387	0	1417	83	0
3	E	38	0	34	0	0
3	H	38	0	34	0	0
3	I	38	0	34	4	0
3	N	38	0	34	8	0
3	O	38	0	34	0	0
4	F	28	0	25	9	0
4	G	28	0	25	2	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	S	28	0	25	7	0
5	A	14	0	13	0	0
5	C	28	0	26	0	0
6	J	50	0	43	0	0
7	K	49	0	43	5	0
8	R	60	0	52	0	0
All	All	10839	0	10492	596	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 28.

The worst 5 of 596 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)
4:F:201:NAG:C6	4:F:203:NAG:H82	1.41	1.46
3:N:401:NAG:C6	3:N:403:NAG:H82	1.54	1.36
4:F:201:NAG:C6	4:F:203:NAG:C8	2.13	1.23
3:N:401:NAG:H61	3:N:403:NAG:C8	1.73	1.19
4:F:201:NAG:H62	4:F:203:NAG:C8	1.72	1.14

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	478/488 (98%)	374 (78%)	74 (16%)	30 (6%)	2	27
1	C	478/488 (98%)	383 (80%)	70 (15%)	25 (5%)	2	31
2	B	178/180 (99%)	125 (70%)	38 (21%)	15 (8%)	1	17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	178/180 (99%)	115 (65%)	45 (25%)	18 (10%)	1	13
All	All	1312/1336 (98%)	997 (76%)	227 (17%)	88 (7%)	1	25

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	30	PRO
1	A	71	ASN
1	A	73	PHE
1	A	118	HIS

### 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	419/443 (95%)	328 (78%)	91 (22%)	1	10
1	C	419/443 (95%)	329 (78%)	90 (22%)	1	10
2	B	154/154 (100%)	123 (80%)	31 (20%)	1	13
2	D	154/154 (100%)	124 (80%)	30 (20%)	2	14
All	All	1146/1194 (96%)	904 (79%)	242 (21%)	1	11

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	130	LEU
1	C	103	SER
2	D	76	GLU
2	B	144	VAL
1	C	8	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	ASN
2	B	178	GLN
2	D	71	HIS
2	B	38	ASN
2	B	54	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 ⓘ

42 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	E	101	1,3	14,14,15	0.58	0	15,19,21	1.09	1 (6%)
3	FUC	E	102	3	10,10,11	0.63	0	14,14,16	2.14	4 (28%)
3	NAG	E	103	3	14,14,15	0.56	0	15,19,21	1.09	0
4	NAG	F	201	1,4	14,14,15	0.58	0	15,19,21	1.01	1 (6%)
4	NAG	F	203	4	14,14,15	0.60	0	15,19,21	1.33	2 (13%)
4	NAG	G	301	1,4	14,14,15	0.53	0	15,19,21	1.26	1 (6%)
4	NAG	G	302	4	14,14,15	0.71	0	15,19,21	1.11	1 (6%)
3	NAG	H	401	1,3	14,14,15	0.47	0	15,19,21	0.89	1 (6%)
3	FUC	H	402	3	10,10,11	0.69	0	14,14,16	1.23	3 (21%)
3	NAG	H	403	3	14,14,15	0.56	0	15,19,21	1.23	1 (6%)
3	NAG	I	501	1,3	14,14,15	0.59	0	15,19,21	1.15	2 (13%)
3	FUC	I	502	3	10,10,11	0.78	0	14,14,16	1.05	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	503	3	14,14,15	0.52	0	15,19,21	0.85	1 (6%)
6	NAG	J	701	1,6	14,14,15	0.68	0	15,19,21	1.27	2 (13%)
6	NAG	J	702	6	14,14,15	0.59	0	15,19,21	1.06	1 (6%)
6	MAN	J	703	6	11,11,12	0.59	0	14,15,17	1.83	3 (21%)
6	MAN	J	704	6	11,11,12	0.56	0	14,15,17	0.93	1 (7%)
7	NAG	K	801	1,7	14,14,15	0.73	0	15,19,21	1.06	0
7	FUC	K	802	7	10,10,11	0.76	0	14,14,16	1.57	2 (14%)
7	NAG	K	803	7	14,14,15	0.51	0	15,19,21	0.85	0
7	MAN	K	804	7	11,11,12	0.72	0	14,15,17	1.44	3 (21%)
4	NAG	L	901	1,4	14,14,15	0.56	0	15,19,21	1.21	2 (13%)
4	NAG	L	902	4	14,14,15	0.45	0	15,19,21	0.91	0
4	NAG	M	101	1,4	14,14,15	0.53	0	15,19,21	1.92	4 (26%)
4	NAG	M	102	4	14,14,15	0.48	0	15,19,21	0.79	0
3	NAG	N	401	1,3	14,14,15	0.50	0	15,19,21	0.83	1 (6%)
3	FUC	N	402	3	10,10,11	0.73	0	14,14,16	1.70	4 (28%)
3	NAG	N	403	3	14,14,15	0.56	0	15,19,21	0.77	0
3	NAG	O	501	1,3	14,14,15	0.56	0	15,19,21	1.01	1 (6%)
3	FUC	O	502	3	10,10,11	0.80	0	14,14,16	1.31	2 (14%)
3	NAG	O	503	3	14,14,15	0.60	0	15,19,21	0.88	1 (6%)
4	NAG	P	601	1,4	14,14,15	0.49	0	15,19,21	1.21	2 (13%)
4	NAG	P	603	4	14,14,15	0.61	0	15,19,21	1.41	2 (13%)
4	NAG	Q	701	1,4	14,14,15	0.49	0	15,19,21	1.83	3 (20%)
4	NAG	Q	703	4	14,14,15	0.83	1 (7%)	15,19,21	1.83	2 (13%)
8	NAG	R	801	1,8	14,14,15	0.78	0	15,19,21	1.61	5 (33%)
8	FUC	R	802	8	10,10,11	0.68	0	14,14,16	1.13	3 (21%)
8	NAG	R	803	8	14,14,15	0.64	0	15,19,21	1.08	2 (13%)
8	MAN	R	804	8	11,11,12	0.88	0	14,15,17	2.19	6 (42%)
8	MAN	R	805	8	11,11,12	0.49	0	14,15,17	2.41	4 (28%)
4	NAG	S	901	1,4	14,14,15	0.44	0	15,19,21	1.65	3 (20%)
4	NAG	S	902	4	14,14,15	0.50	0	15,19,21	1.31	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
3	NAG	E	101	1,3	-	0/6/23/26	0/1/1/1
3	FUC	E	102	3	-	0/0/17/20	0/1/1/1
3	NAG	E	103	3	-	0/6/23/26	0/1/1/1
4	NAG	F	201	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	203	4	-	0/6/23/26	0/1/1/1
4	NAG	G	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	302	4	-	0/6/23/26	0/1/1/1
3	NAG	H	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	402	3	-	0/0/17/20	0/1/1/1
3	NAG	H	403	3	-	0/6/23/26	0/1/1/1
3	NAG	I	501	1,3	-	0/6/23/26	0/1/1/1
3	FUC	I	502	3	-	0/0/17/20	0/1/1/1
3	NAG	I	503	3	-	0/6/23/26	0/1/1/1
6	NAG	J	701	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	702	6	-	0/6/23/26	0/1/1/1
6	MAN	J	703	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	J	704	6	-	0/2/19/22	0/1/1/1
7	NAG	K	801	1,7	-	0/6/23/26	0/1/1/1
7	FUC	K	802	7	-	0/0/17/20	0/1/1/1
7	NAG	K	803	7	-	0/6/23/26	0/1/1/1
7	MAN	K	804	7	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	L	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	902	4	-	0/6/23/26	0/1/1/1
4	NAG	M	101	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	102	4	-	0/6/23/26	0/1/1/1
3	NAG	N	401	1,3	-	0/6/23/26	0/1/1/1
3	FUC	N	402	3	-	0/0/17/20	0/1/1/1
3	NAG	N	403	3	-	0/6/23/26	0/1/1/1
3	NAG	O	501	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	FUC	O	502	3	-	0/0/17/20	0/1/1/1
3	NAG	O	503	3	-	0/6/23/26	0/1/1/1
4	NAG	P	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	603	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	701	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	703	4	-	1/6/23/26	0/1/1/1
8	NAG	R	801	1,8	-	0/6/23/26	0/1/1/1
8	FUC	R	802	8	-	0/0/17/20	0/1/1/1
8	NAG	R	803	8	-	0/6/23/26	0/1/1/1
8	MAN	R	804	8	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	R	805	8	-	0/2/19/22	0/1/1/1
4	NAG	S	901	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	902	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	703	NAG	C1-C2	2.54	1.56	1.52

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	101	NAG	C4-C3-C2	-4.40	104.39	111.23
8	R	804	MAN	C1-O5-C5	-3.81	107.41	112.25
4	L	901	NAG	C2-N2-C7	-3.53	118.51	123.04
3	N	402	FUC	C1-C2-C3	-3.43	105.48	109.54
4	S	902	NAG	C2-N2-C7	-3.33	118.76	123.04

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	R	804	MAN	C1
6	J	703	MAN	C1
3	O	501	NAG	C1
7	K	804	MAN	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	703	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	201	NAG	9	0
4	F	203	NAG	8	0
4	G	301	NAG	2	0
4	G	302	NAG	2	0
3	I	501	NAG	4	0
3	I	502	FUC	4	0
7	K	801	NAG	5	0
7	K	802	FUC	3	0
7	K	803	NAG	2	0
3	N	401	NAG	8	0
3	N	403	NAG	8	0
4	P	601	NAG	1	0
4	P	603	NAG	1	0
4	S	901	NAG	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	902	NAG	6	0

## 5.6 Ligand geometry [i](#)

3 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
5	NAG	A	601	1	14,14,15	0.48	0	15,19,21	1.11	3 (20%)
5	NAG	C	501	1	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
5	NAG	C	601	1	14,14,15	0.45	0	15,19,21	1.46	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
5	NAG	A	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C3-C4-C5	2.05	113.77	110.20
5	A	601	NAG	C4-C3-C2	2.16	114.59	111.23
5	A	601	NAG	C1-O5-C5	2.24	115.09	112.25
5	C	501	NAG	C1-O5-C5	2.58	115.52	112.25
5	C	601	NAG	C1-O5-C5	4.38	117.81	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	480/488 (98%)	-0.58	0 100 100	78, 100, 119, 144	0
1	C	480/488 (98%)	-0.63	0 100 100	80, 100, 119, 141	0
2	B	180/180 (100%)	-0.73	0 100 100	83, 100, 122, 138	0
2	D	180/180 (100%)	-0.74	0 100 100	85, 101, 122, 137	0
All	All	1320/1336 (98%)	-0.64	0 100 100	78, 100, 120, 144	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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
4	NAG	F	201	14/15	0.87	0.41	1.43	90,91,93,95	14
8	NAG	R	801	14/15	0.92	0.20	1.15	80,81,83,83	14
4	NAG	L	901	14/15	0.89	0.26	1.04	85,88,88,89	14
7	NAG	K	801	14/15	0.94	0.22	0.91	56,60,62,64	14
3	NAG	E	101	14/15	0.87	0.23	-	71,74,76,77	14
3	FUC	I	502	10/11	0.87	0.45	-	104,105,106,106	10
3	NAG	N	401	14/15	0.89	0.21	-	96,98,102,102	14

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	Q	703	14/15	0.67	0.40	-	105,107,108,109	14
4	NAG	F	203	14/15	0.76	0.54	-	87,89,90,90	14
8	MAN	R	805	11/12	0.87	0.29	-	67,68,69,69	11
4	NAG	Q	701	14/15	0.81	0.27	-	102,102,104,105	14
3	NAG	N	403	14/15	0.76	0.48	-	103,105,105,105	14
3	FUC	N	402	10/11	0.84	0.36	-	102,103,103,103	10
4	NAG	M	101	14/15	0.89	0.33	-	103,107,108,108	14
8	MAN	R	804	11/12	0.94	0.24	-	68,69,70,71	11
4	NAG	G	302	14/15	0.87	0.37	-	100,101,103,103	14
6	MAN	J	704	11/12	0.84	0.43	-	105,105,106,106	11
3	NAG	I	503	14/15	0.74	0.48	-	114,114,115,115	14
3	NAG	H	401	14/15	0.87	0.24	-	96,98,100,102	14
3	FUC	E	102	10/11	0.89	0.37	-	68,69,69,70	10
4	NAG	G	301	14/15	0.86	0.21	-	92,94,96,98	14
4	NAG	M	102	14/15	0.73	0.56	-	109,109,109,109	14
3	NAG	O	501	14/15	0.83	0.28	-	123,126,130,133	14
7	FUC	K	802	10/11	0.83	0.32	-	57,59,59,59	10
8	NAG	R	803	14/15	0.88	0.28	-	73,78,80,81	14
3	NAG	H	403	14/15	0.65	0.58	-	105,107,108,109	14
4	NAG	S	902	14/15	0.78	0.43	-	96,96,97,97	14
7	MAN	K	804	11/12	0.83	0.36	-	63,64,64,64	11
3	NAG	O	503	14/15	0.74	0.61	-	128,129,129,130	14
8	FUC	R	802	10/11	0.89	0.35	-	83,84,84,84	10
6	MAN	J	703	11/12	0.86	0.39	-	100,101,102,104	11
4	NAG	P	601	14/15	0.82	0.23	-	101,102,105,108	14
7	NAG	K	803	14/15	0.88	0.24	-	59,60,62,63	14
3	NAG	I	501	14/15	0.92	0.26	-	107,112,112,113	14
6	NAG	J	702	14/15	0.84	0.36	-	92,93,95,98	14
4	NAG	P	603	14/15	0.57	0.69	-	110,112,113,113	14
4	NAG	L	902	14/15	0.86	0.37	-	87,87,87,87	14
3	FUC	O	502	10/11	0.51	0.53	-	135,136,137,137	10
4	NAG	S	901	14/15	0.90	0.18	-	92,93,94,95	14
3	NAG	E	103	14/15	0.84	0.38	-	75,76,76,76	14
3	FUC	H	402	10/11	0.84	0.41	-	100,101,101,101	10
6	NAG	J	701	14/15	0.95	0.14	-	81,88,90,90	14

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	501	14/15	0.79	0.38	3.72	89,92,93,94	14
5	NAG	A	601	14/15	0.85	0.29	-	77,86,87,88	14
5	NAG	C	601	14/15	0.85	0.28	-	94,97,99,99	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.