wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:51 AM GMT

PDB ID	:	2J0G
Title	:	L-FICOLIN COMPLEXED TO N-ACETYL-MANNOSAMINE
Authors	:	Garlatti, V.; Gaboriaud, C.
Deposited on	:	2006-08-03
Resolution	:	2.85 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

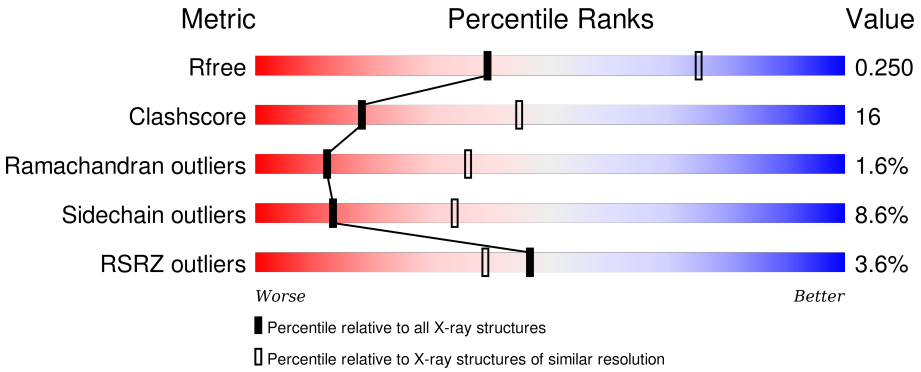
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 >=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 <=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	218	6%, 61%, 33%
1	B	218	72%, 23%
1	C	218	66%, 27%, 6%
1	D	218	14%, 65%, 30%
1	E	218	74%, 23%

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Mol	Chain	Length	Quality of chain
1	F	218	69% 22% 6%

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	BM3	B	400	-	-	X	X
3	BM3	E	400	-	-	-	X
4	MAN	B	1004	X	-	-	-
5	FUC	E	1003	-	-	-	X
5	MAN	E	1004	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10580 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 FICOLIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1702	1071	300	323	8			
1	B	217	Total	C	N	O	S	0	1	0
			1744	1097	307	331	9			
1	C	216	Total	C	N	O	S	0	0	0
			1728	1087	304	328	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	0	0
			1744	1096	307	332	9			
1	F	212	Total	C	N	O	S	0	1	0
			1715	1078	304	325	8			

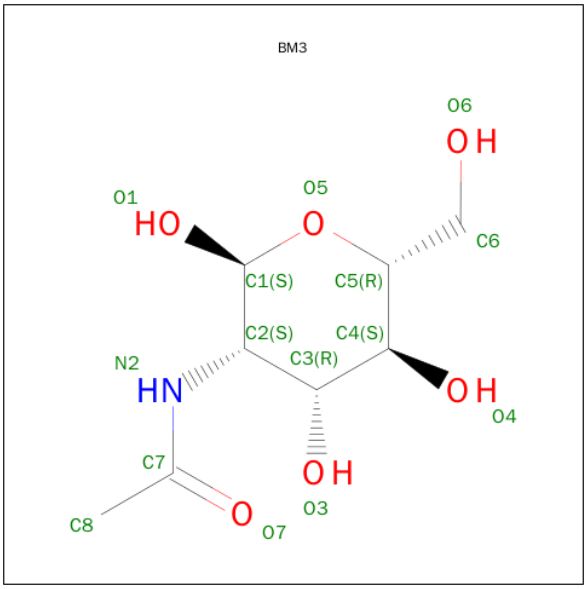
There are 12 discrepancies between the modelled and reference sequences:

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

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

- Molecule 3 is 2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-MANNOPYRANOSE (three-letter code: BM3) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 15 8 1 6	2	0
3	C	1	Total C N O 15 8 1 6	0	0
3	E	1	Total C N O 15 8 1 6	2	0
3	F	1	Total C N O 15 8 1 6	11	0

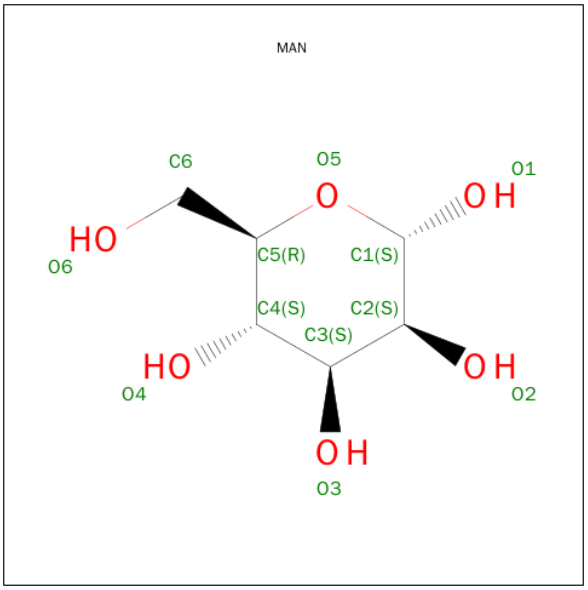
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

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

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

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	B	11	Total	O	0	0
			11	11		
7	C	7	Total	O	0	0
			7	7		
7	D	4	Total	O	0	0
			4	4		

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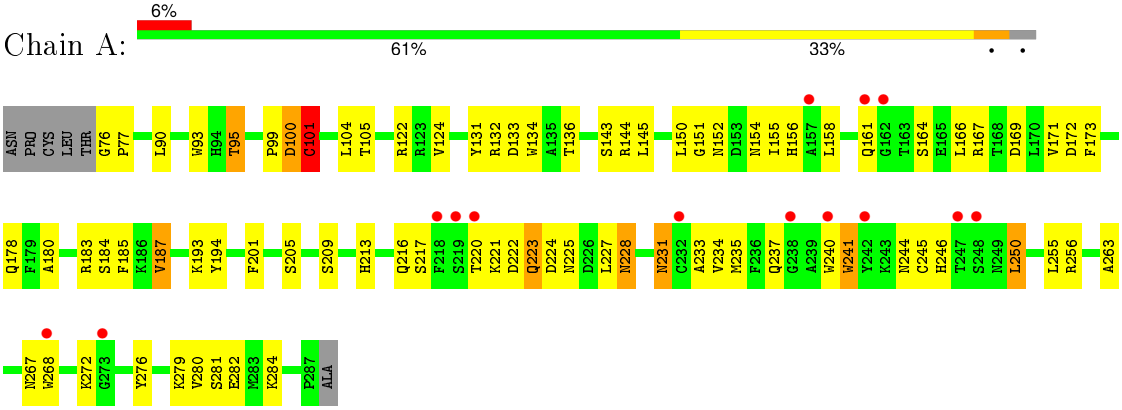
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	9	Total O 9 9	0	0
7	F	10	Total O 10 10	0	0

3 Residue-property plots (i)

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.

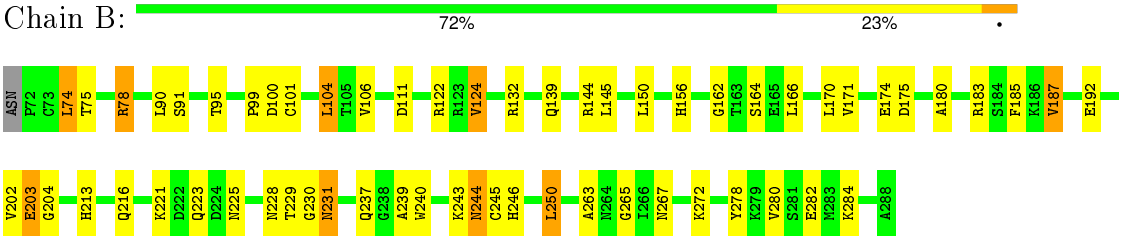
- Molecule 1: FICOLIN-2

Chain A:



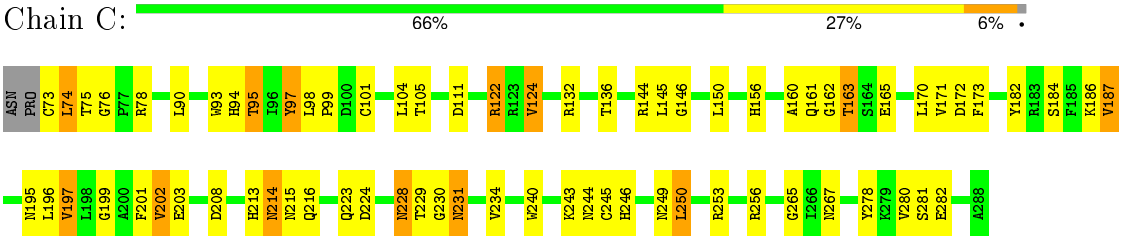
- Molecule 1: FICOLIN-2

Chain B:



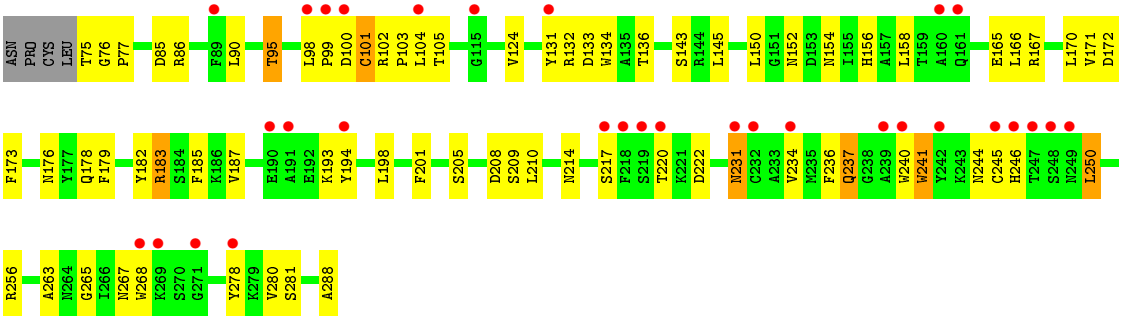
- Molecule 1: FICOLIN-2

Chain C:



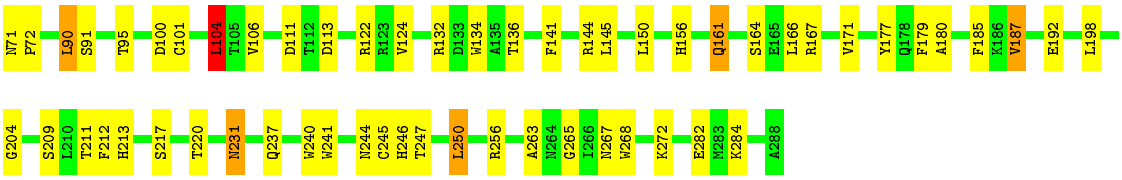
- Molecule 1: FICOLIN-2

Chain D:



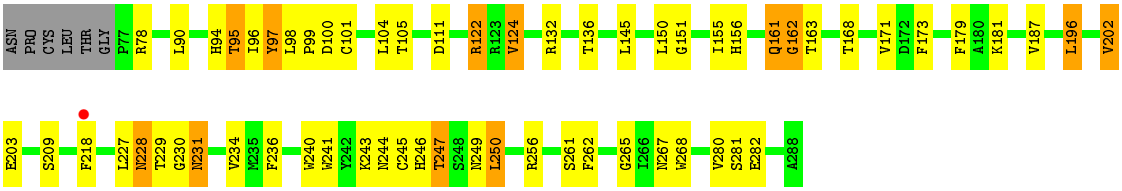
- Molecule 1: FICOLIN-2

Chain E:



- Molecule 1: FICOLIN-2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	96.94Å 96.94Å 139.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.85 48.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.85) 98.9 (48.47-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.72 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.248 0.198 , 0.250	Depositor DCC
R_{free} test set	1681 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.4	EDS
Estimated twinning fraction	0.037 for -h,-k,l 0.447 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 33821 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10580	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BM3, CA, MAN, NAG, FUC

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	0.55	1/1749 (0.1%)	0.66	0/2366
1	B	0.60	0/1792	0.71	0/2423
1	C	0.62	2/1775 (0.1%)	0.69	1/2400 (0.0%)
1	D	0.50	0/1762	0.64	0/2383
1	E	0.56	0/1792	0.71	1/2425 (0.0%)
1	F	0.56	0/1762	0.68	1/2381 (0.0%)
All	All	0.56	3/10632 (0.0%)	0.68	3/14378 (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
4	B	1	0
5	E	1	0
All	All	2	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	GLN	C-N	-11.37	1.07	1.34
1	A	224	ASP	C-N	-8.45	1.14	1.34
1	C	224	ASP	C-N	-6.08	1.20	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	228	ASN	CB-CA-C	-8.89	92.62	110.40
1	C	228	ASN	CB-CA-C	-7.86	94.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	104	LEU	CA-CB-CG	5.61	128.20	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1004	MAN	C1
5	E	1004	MAN	C1

There are no planarity outliers.

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	1702	0	1572	60	0
1	B	1744	0	1613	52	0
1	C	1728	0	1600	55	0
1	D	1715	0	1585	58	0
1	E	1744	0	1611	46	0
1	F	1715	0	1588	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	15	0	14	17	0
3	C	15	0	14	1	0
3	E	15	0	14	3	0
3	F	15	0	14	4	0
4	B	60	0	52	1	0
5	E	49	0	43	1	0
6	F	11	0	10	1	0
7	A	5	0	0	0	0
7	B	11	0	0	1	0
7	C	7	0	0	2	0
7	D	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	9	0	0	0	0
7	F	10	0	0	0	0
All	All	10580	0	9730	318	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 16.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HD2	3:B:400:BM3:C8	1.32	1.53
3:B:400:BM3:C6	3:B:400:BM3:O6	1.75	1.33
3:C:400:BM3:C6	3:C:400:BM3:O6	1.77	1.31
1:B:132:ARG:HD2	3:B:400:BM3:H8C3	1.25	1.14
1:F:132:ARG:HD2	3:F:400:BM3:H8C1	1.22	1.10

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	210/218 (96%)	189 (90%)	18 (9%)	3 (1%)	14	40
1	B	216/218 (99%)	193 (89%)	19 (9%)	4 (2%)	10	32
1	C	214/218 (98%)	190 (89%)	19 (9%)	5 (2%)	8	26
1	D	212/218 (97%)	189 (89%)	19 (9%)	4 (2%)	10	32
1	E	216/218 (99%)	196 (91%)	19 (9%)	1 (0%)	34	67
1	F	211/218 (97%)	185 (88%)	22 (10%)	4 (2%)	10	32
All	All	1279/1308 (98%)	1142 (89%)	116 (9%)	21 (2%)	12	36

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	CYS
1	C	162	GLY
1	F	162	GLY
1	B	162	GLY
1	B	229	THR

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	178/183 (97%)	163 (92%)	15 (8%)	14 35
1	B	183/183 (100%)	163 (89%)	20 (11%)	8 21
1	C	181/183 (99%)	164 (91%)	17 (9%)	11 29
1	D	179/183 (98%)	167 (93%)	12 (7%)	20 47
1	E	183/183 (100%)	170 (93%)	13 (7%)	18 44
1	F	179/183 (98%)	163 (91%)	16 (9%)	12 32
All	All	1083/1098 (99%)	990 (91%)	93 (9%)	13 34

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	150	LEU
1	D	85	ASP
1	F	163	THR
1	C	163	THR
1	C	202	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	195	ASN
1	C	267	ASN

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 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	1001	1,4	14,14,15	0.80	0	15,19,21	1.49	1 (6%)
4	NAG	B	1002	4	14,14,15	0.52	0	15,19,21	1.38	2 (13%)
4	FUC	B	1003	4	10,10,11	0.77	0	14,14,16	1.65	2 (14%)
4	MAN	B	1004	4	11,11,12	0.83	0	14,15,17	1.72	4 (28%)
4	MAN	B	1005	4	11,11,12	0.60	0	14,15,17	1.11	1 (7%)
5	NAG	E	1001	1,5	14,14,15	0.81	1 (7%)	15,19,21	1.24	1 (6%)
5	NAG	E	1002	5	14,14,15	0.68	0	15,19,21	1.20	1 (6%)
5	FUC	E	1003	5	10,10,11	0.89	0	14,14,16	3.19	7 (50%)
5	MAN	E	1004	5,6	11,11,12	0.63	0	14,15,17	1.27	2 (14%)

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	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	4	-	0/6/23/26	0/1/1/1
4	FUC	B	1003	4	-	0/0/17/20	0/1/1/1
4	MAN	B	1004	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	1005	4	-	0/2/19/22	1/1/1/1
5	NAG	E	1001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	1002	5	-	0/6/23/26	0/1/1/1
5	FUC	E	1003	5	-	0/0/17/20	0/1/1/1
5	MAN	E	1004	5,6	1/1/4/5	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1001	NAG	O5-C1	-2.09	1.40	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1003	FUC	C2-C3-C4	-7.73	97.91	111.04
5	E	1003	FUC	C1-C2-C3	-4.59	104.12	109.54
4	B	1001	NAG	C3-C4-C5	-3.92	103.37	110.20
4	B	1004	MAN	O5-C1-C2	-3.48	105.21	110.86
5	E	1004	MAN	C1-O5-C5	-2.36	109.25	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1004	MAN	C1
5	E	1004	MAN	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1005	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1004	MAN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1005	MAN	1	0
5	E	1002	NAG	1	0
5	E	1004	MAN	1	0

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	BM3	B	400	-	15,15,15	3.12	6 (40%)	17,21,21	2.99	8 (47%)
3	BM3	C	400	-	15,15,15	2.61	4 (26%)	17,21,21	3.57	5 (29%)
3	BM3	E	400	-	15,15,15	2.68	3 (20%)	17,21,21	3.08	10 (58%)
3	BM3	F	400	-	15,15,15	3.00	6 (40%)	17,21,21	2.17	4 (23%)
6	MAN	F	402	5	11,11,12	1.42	1 (9%)	14,15,17	1.02	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	BM3	B	400	-	-	0/6/26/26	0/1/1/1
3	BM3	C	400	-	-	0/6/26/26	0/1/1/1
3	BM3	E	400	-	-	0/6/26/26	0/1/1/1
3	BM3	F	400	-	-	1/6/26/26	0/1/1/1
6	MAN	F	402	5	-	0/2/19/22	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	400	BM3	C1-C2	-8.88	1.42	1.53
3	B	400	BM3	C1-C2	-6.54	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	BM3	C1-C2	-4.29	1.48	1.53
3	B	400	BM3	C2-N2	-3.27	1.40	1.45
3	E	400	BM3	O5-C1	-2.35	1.38	1.43

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	400	BM3	C4-C3-C2	-7.43	100.12	110.43
3	C	400	BM3	C4-C3-C2	-7.31	100.29	110.43
3	B	400	BM3	C1-O5-C5	-6.93	100.66	113.47
3	C	400	BM3	C1-O5-C5	-5.74	102.86	113.47
3	B	400	BM3	C4-C3-C2	-5.64	102.61	110.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	400	BM3	C8-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	BM3	17	0
3	C	400	BM3	1	0
3	E	400	BM3	3	0
3	F	400	BM3	4	0
6	F	402	MAN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	212/218 (97%)	0.29	14 (6%) 22 16	33, 39, 50, 55	0
1	B	217/218 (99%)	-0.14	0 100 100	34, 39, 46, 54	0
1	C	216/218 (99%)	-0.05	0 100 100	34, 39, 50, 74	0
1	D	214/218 (98%)	0.62	31 (14%) 3 2	34, 39, 49, 59	0
1	E	218/218 (100%)	-0.15	0 100 100	32, 39, 47, 60	0
1	F	212/218 (97%)	-0.08	1 (0%) 91 90	34, 39, 47, 54	0
All	All	1289/1308 (98%)	0.08	46 (3%) 46 39	32, 39, 48, 74	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	219	SER	7.8
1	D	242	TYR	5.9
1	A	161	GLN	5.2
1	A	242	TYR	5.1
1	D	240	TRP	5.0

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

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

6.3 Carbohydrates

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^{th} 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^2)	Q<0.9
5	FUC	E	1003	10/11	0.64	0.86	35.92	61,63,65,65	0
5	NAG	E	1001	14/15	0.81	0.38	1.84	49,53,59,59	0
4	FUC	B	1003	10/11	0.91	0.25	0.31	52,53,53,54	0
4	NAG	B	1001	14/15	0.97	0.17	-0.96	37,40,49,51	0
5	MAN	E	1004	11/12	0.80	0.27	-	72,73,74,74	0
4	MAN	B	1005	11/12	0.85	0.24	-	88,90,91,91	0
4	NAG	B	1002	14/15	0.96	0.20	-	48,53,57,63	0
5	NAG	E	1002	14/15	0.79	0.41	-	59,63,67,70	0
4	MAN	B	1004	11/12	0.88	0.18	-	68,71,80,85	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
3	BM3	B	400	15/15	0.81	0.39	5.81	32,36,44,48	8
3	BM3	E	400	15/15	0.73	0.37	5.70	27,34,43,45	11
3	BM3	F	400	15/15	0.89	0.24	1.57	29,33,41,42	11
3	BM3	C	400	15/15	0.82	0.24	1.36	28,33,41,42	0
6	MAN	F	402	11/12	0.90	0.23	0.81	20,20,20,20	0
2	CA	F	500	1/1	0.66	0.13	-1.01	46,46,46,46	0
2	CA	B	500	1/1	0.94	0.09	-1.97	27,27,27,27	0
2	CA	C	500	1/1	0.95	0.09	-1.99	38,38,38,38	0
2	CA	A	500	1/1	0.77	0.11	-2.86	75,75,75,75	0
2	CA	E	500	1/1	0.96	0.07	-4.81	34,34,34,34	0
2	CA	D	500	1/1	0.88	0.09	-	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.