WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:38 PM GMT

PDB ID	:	3UEZ
Title	:	Crystal structure of the human Colony-Stimulating Factor 1 (hCSF-1) cytokine in complex with the viral receptor BARF1
Authors	:	Elegheert, J.; Bracke, N.; Savvides, S.N.
Deposited on	:	2011-10-31
Resolution	:	3.41 Å(reported)

The following versions of software and data (see references (i)) 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 3.41 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.
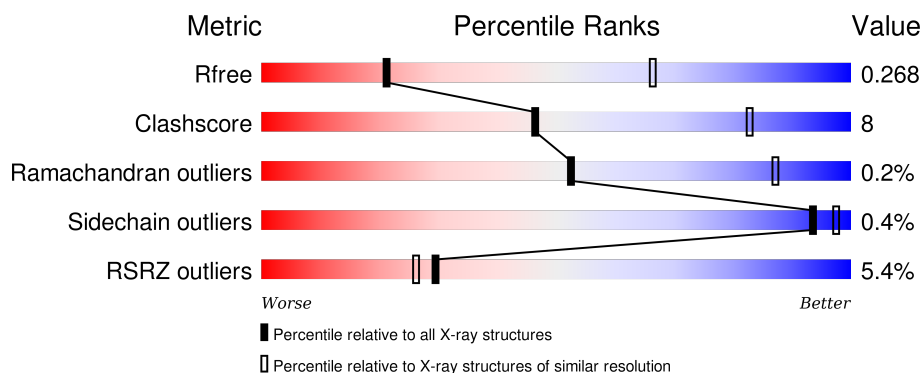
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	208	77% 12% 11%
1	B	208	74% 15% 11%
1	C	208	70% 20% 11%
1	D	208	68% 21% 11%
2	E	153	79% 14% 7%

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Mol	Chain	Length	Quality of chain
2	F	153	16% 75% 17% 8%
2	G	153	4% 80% 13% 7%
2	H	153	14% 71% 20% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10693 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 Secreted protein BARF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total 1477	C 955	N 251	O 264	S 7	0	0	0
1	B	185	Total 1481	C 958	N 252	O 264	S 7	0	0	0
1	C	186	Total 1483	C 958	N 252	O 266	S 7	0	0	0
1	D	186	Total 1487	C 961	N 253	O 266	S 7	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	THR	ENGINEERED MUTATION	UNP P03228
A	222	LYS	-	EXPRESSION TAG	UNP P03228
A	223	HIS	-	EXPRESSION TAG	UNP P03228
A	224	HIS	-	EXPRESSION TAG	UNP P03228
A	225	HIS	-	EXPRESSION TAG	UNP P03228
A	226	HIS	-	EXPRESSION TAG	UNP P03228
A	227	HIS	-	EXPRESSION TAG	UNP P03228
A	228	HIS	-	EXPRESSION TAG	UNP P03228
B	169	SER	THR	ENGINEERED MUTATION	UNP P03228
B	222	LYS	-	EXPRESSION TAG	UNP P03228
B	223	HIS	-	EXPRESSION TAG	UNP P03228
B	224	HIS	-	EXPRESSION TAG	UNP P03228
B	225	HIS	-	EXPRESSION TAG	UNP P03228
B	226	HIS	-	EXPRESSION TAG	UNP P03228
B	227	HIS	-	EXPRESSION TAG	UNP P03228
B	228	HIS	-	EXPRESSION TAG	UNP P03228
C	169	SER	THR	ENGINEERED MUTATION	UNP P03228
C	222	LYS	-	EXPRESSION TAG	UNP P03228
C	223	HIS	-	EXPRESSION TAG	UNP P03228
C	224	HIS	-	EXPRESSION TAG	UNP P03228
C	225	HIS	-	EXPRESSION TAG	UNP P03228

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Chain	Residue	Modelled	Actual	Comment	Reference
C	226	HIS	-	EXPRESSION TAG	UNP P03228
C	227	HIS	-	EXPRESSION TAG	UNP P03228
C	228	HIS	-	EXPRESSION TAG	UNP P03228
D	169	SER	THR	ENGINEERED MUTATION	UNP P03228
D	222	LYS	-	EXPRESSION TAG	UNP P03228
D	223	HIS	-	EXPRESSION TAG	UNP P03228
D	224	HIS	-	EXPRESSION TAG	UNP P03228
D	225	HIS	-	EXPRESSION TAG	UNP P03228
D	226	HIS	-	EXPRESSION TAG	UNP P03228
D	227	HIS	-	EXPRESSION TAG	UNP P03228
D	228	HIS	-	EXPRESSION TAG	UNP P03228

- Molecule 2 is a protein called Macrophage colony-stimulating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	142	Total 1159	C 730	N 193	O 225	S 11	0	0	0
2	F	141	Total 1150	C 723	N 192	O 224	S 11	0	0	0
2	G	143	Total 1174	C 739	N 195	O 229	S 11	0	1	0
2	H	139	Total 1126	C 708	N 189	O 218	S 11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P09603
E	-2	SER	-	EXPRESSION TAG	UNP P09603
E	-1	HIS	-	EXPRESSION TAG	UNP P09603
E	0	MET	-	EXPRESSION TAG	UNP P09603
F	-3	GLY	-	EXPRESSION TAG	UNP P09603
F	-2	SER	-	EXPRESSION TAG	UNP P09603
F	-1	HIS	-	EXPRESSION TAG	UNP P09603
F	0	MET	-	EXPRESSION TAG	UNP P09603
G	-3	GLY	-	EXPRESSION TAG	UNP P09603
G	-2	SER	-	EXPRESSION TAG	UNP P09603
G	-1	HIS	-	EXPRESSION TAG	UNP P09603
G	0	MET	-	EXPRESSION TAG	UNP P09603
H	-3	GLY	-	EXPRESSION TAG	UNP P09603
H	-2	SER	-	EXPRESSION TAG	UNP P09603
H	-1	HIS	-	EXPRESSION TAG	UNP P09603

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	EXPRESSION TAG	UNP P09603

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

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

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: Secreted protein BARF1

Chain A:

- Molecule 1: Secreted protein BARF1

Chain B:

- Molecule 1: Secreted protein BARF1

Chain C:

- Molecule 1: Secreted protein BARF1

Chain D:

M160 PRO GLU GLY VAL GLU PRO ALA PRO SER ALA ALA ASN GLY GLY V175 V185 L189 K193 P194 V199 K204 N205 E208 L219 S220 GLN LYS HIS HIS HIS HIS HIS

- Molecule 2: Macrophage colony-stimulating factor 1
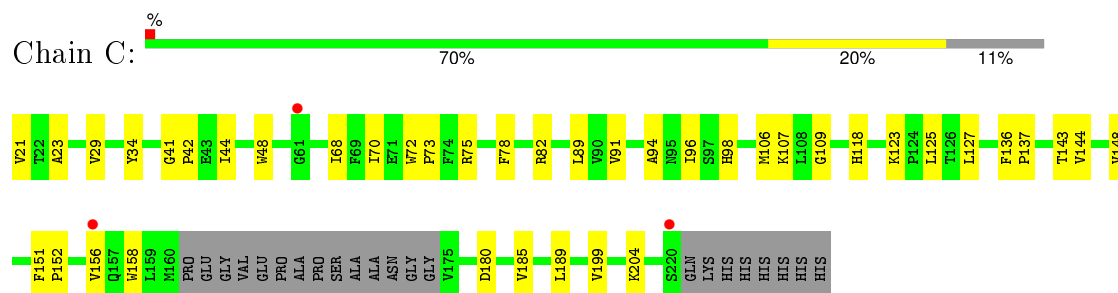
Chain E:

7%

79% 14% 7%

GLY SER HIS MET GLU GLU VAL SER GLU Y6 C7 S8 I11 G12 S13 S18 L22 Q26 T34 F37 Q40 K44 K51 K52 E62 D63 R66 D94 Y95 D99 K100 A101 R104 T105 F106 N119 M122 E123 T124 I134 F135 S136 K137

F143 S147 SER GLN

- Molecule 2: Macrophage colony-stimulating factor 1

Chain F:

16%

75% 17% 8%

GLY SER HIS MET GLU GLU VAL SER E5 S13 Q17 R21 L22 F35 E36 F37 D45 P46 K52 L55 L56 E62 D63 T64 N73 I77 C90 D94 TYR E96 E97 H98 D99 K100 A101 C102 V103 R104 T105 F106 L113 N119 M122 E123

N126 L127 L128 W132 N133 I134 F135 S136 K137 N138 C139 N140 N141 S142 F143 A144 E145 C146 SER SER GLN

- Molecule 2: Macrophage colony-stimulating factor 1

Chain G:

4%

80% 13% 7%

GLY SER HIS MET GLU GLU VAL S4 E5 M10 S25 T34 F37 L43 K52 M65 L87 D99 K100 A101 C102 V103 R104 T105 F106 V117 K118 N119 E123 T124 W132 N133 S142 C146 SER SER GLN

- Molecule 2: Macrophage colony-stimulating factor 1

Chain H:

14%

71% 20% 9%

GLY SER HIS MET GLU GLU VAL SER GLU TYR C7 S8 H9 M10 I11 S25 T34 F35 E36 F37 V38 V47 A53 F54 L55 L56 V57 Q58 D59 I60 M61 E62 D63 T64 M65 R66 F67 R68 I77 V78 Q79 L80 Q81 L85 R86 L87 C90 D94 TYR E96 E97 H98

D99 K100 V103 R104 T105 T109 P110 L113 V117 K118 N119 E123 N126 L127 L128 D129 N138 C139 N140 N141 S142 F143 C146 SER SER GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	235.24Å 235.24Å 95.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.41 58.81 – 3.41	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-3.41) 96.4 (58.81-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_874)	Depositor
R, R_{free}	0.231 , 0.274 0.219 , 0.268	Depositor DCC
R_{free} test set	1295 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 22.8	EDS
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.45$, $<L^2> = 0.27$	Xtriage
Outliers	0 of 25861 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10693	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.22	0/1520	0.41	0/2069
1	B	0.22	0/1524	0.41	0/2073
1	C	0.23	0/1526	0.41	0/2077
1	D	0.22	0/1530	0.40	0/2081
2	E	0.22	0/1179	0.36	0/1589
2	F	0.22	0/1168	0.37	0/1572
2	G	0.23	0/1197	0.36	0/1613
2	H	0.22	0/1143	0.37	0/1538
All	All	0.22	0/10787	0.39	0/14612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1477	0	1445	16	0
1	B	1481	0	1456	18	0
1	C	1483	0	1450	29	0
1	D	1487	0	1461	25	0
2	E	1159	0	1122	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1150	0	1113	20	0
2	G	1174	0	1136	17	0
2	H	1126	0	1094	26	0
3	A	39	0	34	1	0
3	B	39	0	34	0	0
3	C	39	0	34	0	0
3	D	39	0	34	0	0
All	All	10693	0	10413	161	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 8.

The worst 5 of 161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:GLU:N	2:F:5:GLU:OE1	2.29	0.65
2:G:52:LYS:NZ	2:G:101:ALA:O	2.32	0.63
2:E:51:LYS:NZ	2:E:137:LYS:O	2.34	0.61
1:C:70:ILE:O	1:C:75:ARG:NH1	2.35	0.59
2:F:134:ILE:HG23	2:F:135:PHE:CD2	2.39	0.57

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	181/208 (87%)	177 (98%)	4 (2%)	0	100	100
1	B	181/208 (87%)	173 (96%)	7 (4%)	1 (1%)	30	73
1	C	182/208 (88%)	178 (98%)	3 (2%)	1 (0%)	34	75
1	D	182/208 (88%)	174 (96%)	7 (4%)	1 (0%)	34	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	F	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
2	G	142/153 (93%)	139 (98%)	3 (2%)	0	100	100
2	H	135/153 (88%)	128 (95%)	7 (5%)	0	100	100
All	All	1280/1444 (89%)	1238 (97%)	39 (3%)	3 (0%)	52	87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	D	41	GLY
1	C	41	GLY

5.3.2 Protein sidechains (i)

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	165/183 (90%)	165 (100%)	0	100	100
1	B	166/183 (91%)	165 (99%)	1 (1%)	90	96
1	C	166/183 (91%)	165 (99%)	1 (1%)	90	96
1	D	167/183 (91%)	165 (99%)	2 (1%)	78	91
2	E	134/145 (92%)	134 (100%)	0	100	100
2	F	133/145 (92%)	133 (100%)	0	100	100
2	G	136/145 (94%)	136 (100%)	0	100	100
2	H	130/145 (90%)	129 (99%)	1 (1%)	86	95
All	All	1197/1312 (91%)	1192 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	LYS

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Mol	Chain	Res	Type
1	C	204	LYS
1	D	110	GLU
1	D	193	LYS
2	H	90	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	HIS
1	C	57	GLN
1	B	118	HIS
1	A	101	ASN
1	B	130	HIS

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)

12 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	300	1,3	14,14,15	0.47	0	15,19,21	0.88	1 (6%)
3	NAG	A	301	3	14,14,15	0.47	0	15,19,21	0.84	0
3	BMA	A	302	3	11,11,12	0.59	0	14,15,17	0.69	0
3	NAG	B	300	1,3	14,14,15	0.64	0	15,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAG	B	301	3	14,14,15	0.47	0	15,19,21	0.66	0
3	BMA	B	302	3	11,11,12	0.58	0	14,15,17	0.76	0
3	NAG	C	300	1,3	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
3	NAG	C	301	3	14,14,15	0.48	0	15,19,21	0.67	0
3	BMA	C	302	3	11,11,12	0.56	0	14,15,17	0.76	0
3	NAG	D	300	1,3	14,14,15	0.61	0	15,19,21	1.06	1 (6%)
3	NAG	D	301	3	14,14,15	0.53	0	15,19,21	0.82	0
3	BMA	D	302	3	11,11,12	0.61	0	14,15,17	1.16	1 (7%)

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	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	301	3	-	0/6/23/26	0/1/1/1
3	BMA	A	302	3	-	0/2/19/22	0/1/1/1
3	NAG	B	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	301	3	-	0/6/23/26	0/1/1/1
3	BMA	B	302	3	-	0/2/19/22	0/1/1/1
3	NAG	C	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	301	3	-	0/6/23/26	0/1/1/1
3	BMA	C	302	3	-	0/2/19/22	0/1/1/1
3	NAG	D	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	301	3	-	0/6/23/26	0/1/1/1
3	BMA	D	302	3	-	0/2/19/22	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(^{o})	Ideal(^{o})
3	A	300	NAG	C1-O5-C5	2.19	115.03	112.25
3	B	300	NAG	C4-C3-C2	2.38	114.94	111.23
3	D	300	NAG	C4-C3-C2	3.07	116.00	111.23
3	C	300	NAG	C1-O5-C5	3.33	116.47	112.25
3	D	302	BMA	C1-C2-C3	3.76	113.99	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAG	1	0
3	A	302	BMA	1	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, 95th 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	185/208 (88%)	0.23	2 (1%)	82	76	45, 60, 81, 94	0
1	B	185/208 (88%)	0.23	1 (0%)	91	89	46, 64, 80, 102	0
1	C	186/208 (89%)	0.15	3 (1%)	74	69	50, 63, 89, 108	0
1	D	186/208 (89%)	0.17	1 (0%)	91	89	45, 62, 85, 115	0
2	E	142/153 (92%)	0.43	10 (7%)	19	18	57, 85, 111, 119	0
2	F	141/153 (92%)	0.97	25 (17%)	2	2	61, 105, 153, 170	0
2	G	143/153 (93%)	0.29	6 (4%)	40	35	62, 90, 113, 138	0
2	H	139/153 (90%)	0.97	22 (15%)	3	3	56, 110, 148, 168	0
All	All	1307/1444 (90%)	0.40	70 (5%)	29	26	45, 72, 133, 170	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	133	ASN	8.0
2	H	79	GLN	6.5
2	H	138	ASN	5.5
2	F	136	SER	5.3
2	F	132	TRP	4.6

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.

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The B-factors column lists the minimum, median, 95th 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	NAG	C	300	14/15	0.94	0.16	-0.65	50,65,72,74	0
3	NAG	D	300	14/15	0.96	0.18	-0.66	50,62,66,68	0
3	NAG	A	300	14/15	0.93	0.19	-0.77	49,61,70,78	0
3	NAG	B	300	14/15	0.94	0.15	-1.82	42,60,63,69	0
3	NAG	A	301	14/15	0.92	0.23	-	63,70,80,81	0
3	BMA	D	302	11/12	0.82	0.20	-	70,80,91,97	0
3	BMA	A	302	11/12	0.84	0.17	-	74,80,89,91	0
3	BMA	C	302	11/12	0.82	0.18	-	71,80,88,93	0
3	BMA	B	302	11/12	0.69	0.37	-	67,75,94,96	0
3	NAG	B	301	14/15	0.91	0.22	-	60,64,70,71	0
3	NAG	D	301	14/15	0.95	0.14	-	52,64,80,85	0
3	NAG	C	301	14/15	0.93	0.16	-	61,68,72,73	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.