



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:21 am GMT

PDB ID : 4ADF  
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 : 2011-12-23  
Resolution : 4.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

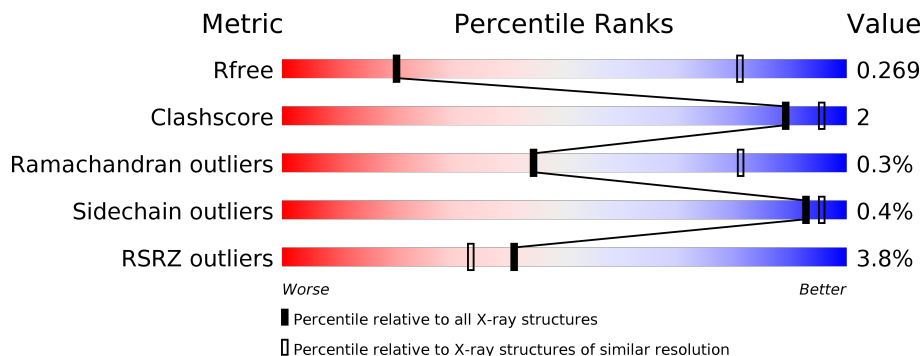
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










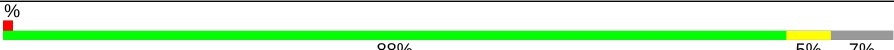
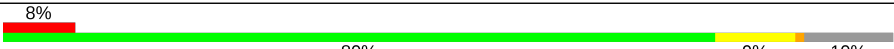

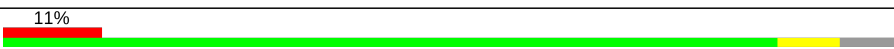




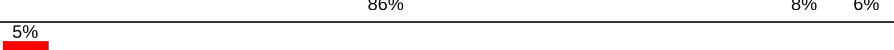
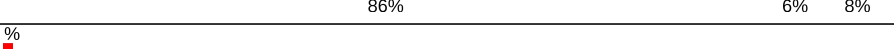

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1024 (5.08-3.62)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1007 (5.08-3.64)

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	208	
1	B	208	
1	C	208	
1	D	208	
1	E	208	
1	F	208	

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Mol	Chain	Length	Quality of chain
1	M	208	
1	N	208	
1	O	208	
1	P	208	
1	Q	208	
1	R	208	
2	G	153	
2	H	153	
2	I	153	
2	J	153	
2	K	153	
2	L	153	
2	S	153	
2	T	153	
2	U	153	
2	V	153	
2	W	153	
2	X	153	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32413 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	188	Total	C	N	O	S	0	0	0
			1494	965	255	267	7			
1	B	189	Total	C	N	O	S	0	0	0
			1498	967	255	269	7			
1	C	186	Total	C	N	O	S	0	0	0
			1481	956	253	265	7			
1	D	187	Total	C	N	O	S	0	0	0
			1487	960	253	267	7			
1	E	187	Total	C	N	O	S	0	0	0
			1485	959	253	266	7			
1	F	189	Total	C	N	O	S	0	0	0
			1495	965	255	268	7			
1	M	191	Total	C	N	O	S	0	0	0
			1507	973	257	270	7			
1	N	191	Total	C	N	O	S	0	0	0
			1517	978	259	273	7			
1	O	186	Total	C	N	O	S	0	0	0
			1476	954	250	265	7			
1	P	189	Total	C	N	O	S	0	0	0
			1502	970	256	269	7			
1	Q	185	Total	C	N	O	S	0	0	0
			1481	958	252	264	7			
1	R	186	Total	C	N	O	S	0	0	0
			1483	958	252	266	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	-	EXPRESSION TAG	UNP P0CW72
A	223	HIS	-	EXPRESSION TAG	UNP P0CW72
A	224	HIS	-	EXPRESSION TAG	UNP P0CW72
A	225	HIS	-	EXPRESSION TAG	UNP P0CW72
A	226	HIS	-	EXPRESSION TAG	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	-	EXPRESSION TAG	UNP P0CW72
A	228	HIS	-	EXPRESSION TAG	UNP P0CW72
A	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
B	222	LYS	-	EXPRESSION TAG	UNP P0CW72
B	223	HIS	-	EXPRESSION TAG	UNP P0CW72
B	224	HIS	-	EXPRESSION TAG	UNP P0CW72
B	225	HIS	-	EXPRESSION TAG	UNP P0CW72
B	226	HIS	-	EXPRESSION TAG	UNP P0CW72
B	227	HIS	-	EXPRESSION TAG	UNP P0CW72
B	228	HIS	-	EXPRESSION TAG	UNP P0CW72
B	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
C	222	LYS	-	EXPRESSION TAG	UNP P0CW72
C	223	HIS	-	EXPRESSION TAG	UNP P0CW72
C	224	HIS	-	EXPRESSION TAG	UNP P0CW72
C	225	HIS	-	EXPRESSION TAG	UNP P0CW72
C	226	HIS	-	EXPRESSION TAG	UNP P0CW72
C	227	HIS	-	EXPRESSION TAG	UNP P0CW72
C	228	HIS	-	EXPRESSION TAG	UNP P0CW72
C	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
D	222	LYS	-	EXPRESSION TAG	UNP P0CW72
D	223	HIS	-	EXPRESSION TAG	UNP P0CW72
D	224	HIS	-	EXPRESSION TAG	UNP P0CW72
D	225	HIS	-	EXPRESSION TAG	UNP P0CW72
D	226	HIS	-	EXPRESSION TAG	UNP P0CW72
D	227	HIS	-	EXPRESSION TAG	UNP P0CW72
D	228	HIS	-	EXPRESSION TAG	UNP P0CW72
D	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
E	222	LYS	-	EXPRESSION TAG	UNP P0CW72
E	223	HIS	-	EXPRESSION TAG	UNP P0CW72
E	224	HIS	-	EXPRESSION TAG	UNP P0CW72
E	225	HIS	-	EXPRESSION TAG	UNP P0CW72
E	226	HIS	-	EXPRESSION TAG	UNP P0CW72
E	227	HIS	-	EXPRESSION TAG	UNP P0CW72
E	228	HIS	-	EXPRESSION TAG	UNP P0CW72
E	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
F	222	LYS	-	EXPRESSION TAG	UNP P0CW72
F	223	HIS	-	EXPRESSION TAG	UNP P0CW72
F	224	HIS	-	EXPRESSION TAG	UNP P0CW72
F	225	HIS	-	EXPRESSION TAG	UNP P0CW72
F	226	HIS	-	EXPRESSION TAG	UNP P0CW72
F	227	HIS	-	EXPRESSION TAG	UNP P0CW72
F	228	HIS	-	EXPRESSION TAG	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
F	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
M	222	LYS	-	EXPRESSION TAG	UNP P0CW72
M	223	HIS	-	EXPRESSION TAG	UNP P0CW72
M	224	HIS	-	EXPRESSION TAG	UNP P0CW72
M	225	HIS	-	EXPRESSION TAG	UNP P0CW72
M	226	HIS	-	EXPRESSION TAG	UNP P0CW72
M	227	HIS	-	EXPRESSION TAG	UNP P0CW72
M	228	HIS	-	EXPRESSION TAG	UNP P0CW72
M	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
N	222	LYS	-	EXPRESSION TAG	UNP P0CW72
N	223	HIS	-	EXPRESSION TAG	UNP P0CW72
N	224	HIS	-	EXPRESSION TAG	UNP P0CW72
N	225	HIS	-	EXPRESSION TAG	UNP P0CW72
N	226	HIS	-	EXPRESSION TAG	UNP P0CW72
N	227	HIS	-	EXPRESSION TAG	UNP P0CW72
N	228	HIS	-	EXPRESSION TAG	UNP P0CW72
N	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
O	222	LYS	-	EXPRESSION TAG	UNP P0CW72
O	223	HIS	-	EXPRESSION TAG	UNP P0CW72
O	224	HIS	-	EXPRESSION TAG	UNP P0CW72
O	225	HIS	-	EXPRESSION TAG	UNP P0CW72
O	226	HIS	-	EXPRESSION TAG	UNP P0CW72
O	227	HIS	-	EXPRESSION TAG	UNP P0CW72
O	228	HIS	-	EXPRESSION TAG	UNP P0CW72
O	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
P	222	LYS	-	EXPRESSION TAG	UNP P0CW72
P	223	HIS	-	EXPRESSION TAG	UNP P0CW72
P	224	HIS	-	EXPRESSION TAG	UNP P0CW72
P	225	HIS	-	EXPRESSION TAG	UNP P0CW72
P	226	HIS	-	EXPRESSION TAG	UNP P0CW72
P	227	HIS	-	EXPRESSION TAG	UNP P0CW72
P	228	HIS	-	EXPRESSION TAG	UNP P0CW72
P	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
Q	222	LYS	-	EXPRESSION TAG	UNP P0CW72
Q	223	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	224	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	225	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	226	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	227	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	228	HIS	-	EXPRESSION TAG	UNP P0CW72
Q	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72
R	222	LYS	-	EXPRESSION TAG	UNP P0CW72

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Chain	Residue	Modelled	Actual	Comment	Reference
R	223	HIS	-	EXPRESSION TAG	UNP P0CW72
R	224	HIS	-	EXPRESSION TAG	UNP P0CW72
R	225	HIS	-	EXPRESSION TAG	UNP P0CW72
R	226	HIS	-	EXPRESSION TAG	UNP P0CW72
R	227	HIS	-	EXPRESSION TAG	UNP P0CW72
R	228	HIS	-	EXPRESSION TAG	UNP P0CW72
R	169	SER	THR	ENGINEERED MUTATION	UNP P0CW72

- Molecule 2 is a protein called MACROPHAGE COLONY-STIMULATING FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	145	Total	C	N	O	S	0	0	0
			1161	729	193	228	11			
2	H	142	Total	C	N	O	S	0	0	0
			1145	722	192	220	11			
2	I	137	Total	C	N	O	S	0	0	0
			1097	690	182	214	11			
2	J	142	Total	C	N	O	S	0	0	0
			1149	723	192	223	11			
2	K	143	Total	C	N	O	S	0	0	0
			1157	726	193	227	11			
2	L	135	Total	C	N	O	S	0	0	0
			1089	686	183	209	11			
2	S	144	Total	C	N	O	S	0	0	0
			1157	726	190	230	11			
2	T	142	Total	C	N	O	S	0	0	0
			1148	723	191	223	11			
2	U	144	Total	C	N	O	S	0	0	0
			1159	727	194	227	11			
2	V	141	Total	C	N	O	S	0	0	0
			1140	719	192	218	11			
2	W	142	Total	C	N	O	S	0	0	0
			1128	710	188	219	11			
2	X	139	Total	C	N	O	S	0	0	0
			1113	702	183	217	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	EXPRESSION TAG	UNP P09603
G	-2	SER	-	EXPRESSION TAG	UNP P09603
G	-1	HIS	-	EXPRESSION TAG	UNP P09603

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Chain	Residue	Modelled	Actual	Comment	Reference
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
H	0	MET	-	EXPRESSION TAG	UNP P09603
I	-3	GLY	-	EXPRESSION TAG	UNP P09603
I	-2	SER	-	EXPRESSION TAG	UNP P09603
I	-1	HIS	-	EXPRESSION TAG	UNP P09603
I	0	MET	-	EXPRESSION TAG	UNP P09603
J	-3	GLY	-	EXPRESSION TAG	UNP P09603
J	-2	SER	-	EXPRESSION TAG	UNP P09603
J	-1	HIS	-	EXPRESSION TAG	UNP P09603
J	0	MET	-	EXPRESSION TAG	UNP P09603
K	-3	GLY	-	EXPRESSION TAG	UNP P09603
K	-2	SER	-	EXPRESSION TAG	UNP P09603
K	-1	HIS	-	EXPRESSION TAG	UNP P09603
K	0	MET	-	EXPRESSION TAG	UNP P09603
L	-3	GLY	-	EXPRESSION TAG	UNP P09603
L	-2	SER	-	EXPRESSION TAG	UNP P09603
L	-1	HIS	-	EXPRESSION TAG	UNP P09603
L	0	MET	-	EXPRESSION TAG	UNP P09603
S	-3	GLY	-	EXPRESSION TAG	UNP P09603
S	-2	SER	-	EXPRESSION TAG	UNP P09603
S	-1	HIS	-	EXPRESSION TAG	UNP P09603
S	0	MET	-	EXPRESSION TAG	UNP P09603
T	-3	GLY	-	EXPRESSION TAG	UNP P09603
T	-2	SER	-	EXPRESSION TAG	UNP P09603
T	-1	HIS	-	EXPRESSION TAG	UNP P09603
T	0	MET	-	EXPRESSION TAG	UNP P09603
U	-3	GLY	-	EXPRESSION TAG	UNP P09603
U	-2	SER	-	EXPRESSION TAG	UNP P09603
U	-1	HIS	-	EXPRESSION TAG	UNP P09603
U	0	MET	-	EXPRESSION TAG	UNP P09603
V	-3	GLY	-	EXPRESSION TAG	UNP P09603
V	-2	SER	-	EXPRESSION TAG	UNP P09603
V	-1	HIS	-	EXPRESSION TAG	UNP P09603
V	0	MET	-	EXPRESSION TAG	UNP P09603
W	-3	GLY	-	EXPRESSION TAG	UNP P09603
W	-2	SER	-	EXPRESSION TAG	UNP P09603
W	-1	HIS	-	EXPRESSION TAG	UNP P09603
W	0	MET	-	EXPRESSION TAG	UNP P09603
X	-3	GLY	-	EXPRESSION TAG	UNP P09603

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	SER	-	EXPRESSION TAG	UNP P09603
X	-1	HIS	-	EXPRESSION TAG	UNP P09603
X	0	MET	-	EXPRESSION TAG	UNP P09603

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		
3	M	6	Total	C	N	O	0	0
			72	40	2	30		
3	N	6	Total	C	N	O	0	0
			72	40	2	30		
3	P	6	Total	C	N	O	0	0
			72	40	2	30		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	7	Total	C	N	O	0	0
			83	46	2	35		
4	C	7	Total	C	N	O	0	0
			83	46	2	35		
4	Q	7	Total	C	N	O	0	0
			83	46	2	35		
4	R	7	Total	C	N	O	0	0
			83	46	2	35		


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

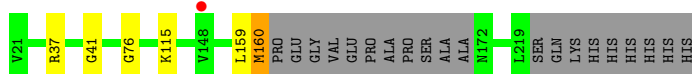
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	5	Total	C	N	O	0	0
			61	34	2	25		
5	E	5	Total	C	N	O	0	0
			61	34	2	25		
5	F	5	Total	C	N	O	0	0
			61	34	2	25		
5	O	5	Total	C	N	O	0	0
			61	34	2	25		

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

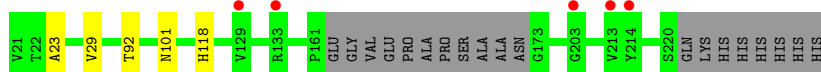
#### • Molecule 1: SECRETED PROTEIN BARF1

Chain A:  88% 10%




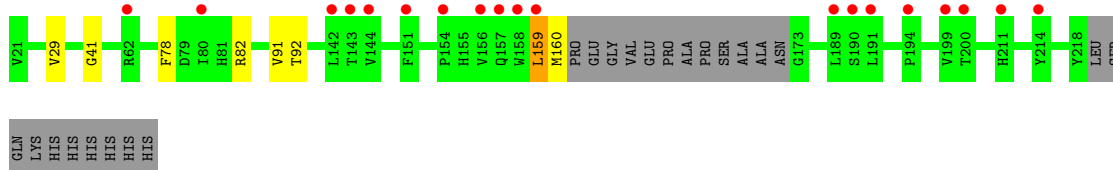
#### • Molecule 1: SECRETED PROTEIN BARF1

Chain B:  88% 9%




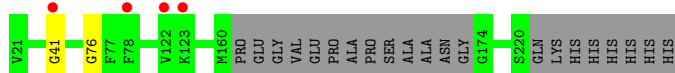
#### • Molecule 1: SECRETED PROTEIN BARF1

Chain C:  86% 11%




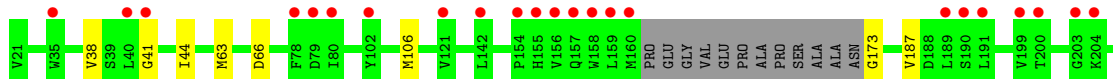
#### • Molecule 1: SECRETED PROTEIN BARF1

Chain D:  89% 10%




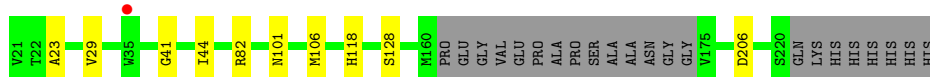
#### • Molecule 1: SECRETED PROTEIN BARF1

Chain E:  86% 10%






Chain R: 




• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain G: 




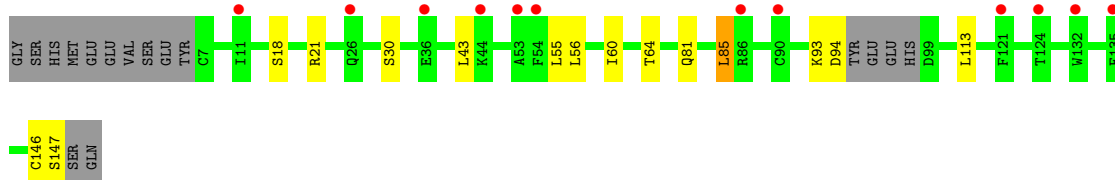
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain H: 




• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain I: 




• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain J: 




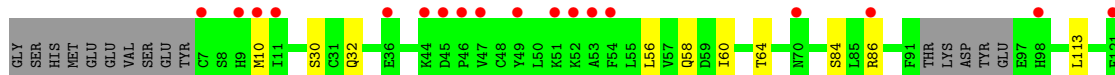
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

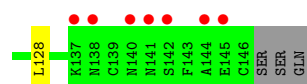
Chain K: 



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain L: 





• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain S: 85% 9% 6%



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain T: 2% 89% 7%



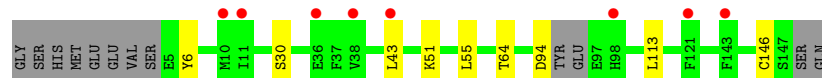
• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain U: 86% 8% 6%



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain V: 5% 86% 6% 8%



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain W: 0% 85% 7% 7%



• Molecule 2: MACROPHAGE COLONY-STIMULATING FACTOR 1

Chain X: 0% 86% 5% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.44Å 218.44Å 331.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.85 – 4.40 75.85 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.85-4.40) 99.2 (75.85-4.40)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 4.46Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.238 , 0.276 0.233 , 0.269	Depositor DCC
$R_{free}$ test set	2869 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	165.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 182.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	32413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	216.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.31	0/1537	0.65	2/2090 (0.1%)
1	B	0.30	0/1542	0.57	0/2099
1	C	0.31	0/1524	0.60	1/2072 (0.0%)
1	D	0.30	0/1530	0.58	0/2082
1	E	0.30	0/1528	0.56	0/2079
1	F	0.34	0/1538	0.63	1/2093 (0.0%)
1	M	0.33	0/1551	0.63	0/2112
1	N	0.33	0/1561	0.63	0/2123
1	O	0.31	0/1520	0.62	0/2073
1	P	0.32	0/1546	0.58	0/2103
1	Q	0.31	0/1524	0.60	0/2073
1	R	0.32	0/1526	0.61	0/2077
2	G	0.33	0/1179	0.66	0/1591
2	H	0.35	0/1164	0.67	0/1568
2	I	0.31	0/1113	0.63	0/1500
2	J	0.31	0/1168	0.61	1/1574 (0.1%)
2	K	0.30	0/1176	0.58	0/1586
2	L	0.32	0/1106	0.63	1/1490 (0.1%)
2	S	0.32	0/1176	0.64	0/1589
2	T	0.34	0/1166	0.63	0/1570
2	U	0.33	0/1178	0.69	0/1589
2	V	0.30	0/1158	0.62	3/1558 (0.2%)
2	W	0.34	0/1145	0.70	1/1546 (0.1%)
2	X	0.35	0/1130	0.64	0/1523
All	All	0.32	0/32286	0.62	10/43760 (0.0%)

There are no bond length outliers.

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	MET	CA-CB-CG	8.81	128.28	113.30
2	W	75	ILE	CG1-CB-CG2	-5.90	98.43	111.40
2	V	6	TYR	CB-CG-CD1	5.43	124.26	121.00
2	L	128	LEU	CA-CB-CG	5.34	127.59	115.30
2	J	128	LEU	CA-CB-CG	5.34	127.59	115.30

There are no chirality outliers.

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	1494	0	1464	3	0
1	B	1498	0	1463	4	0
1	C	1481	0	1451	6	0
1	D	1487	0	1453	1	0
1	E	1485	0	1451	4	0
1	F	1495	0	1458	5	0
1	M	1507	0	1470	10	0
1	N	1517	0	1484	15	0
1	O	1476	0	1430	7	0
1	P	1502	0	1474	9	0
1	Q	1481	0	1456	8	0
1	R	1483	0	1450	7	0
2	G	1161	0	1115	8	0
2	H	1145	0	1112	4	0
2	I	1097	0	1062	9	0
2	J	1149	0	1111	4	0
2	K	1157	0	1110	7	0
2	L	1089	0	1053	5	0
2	S	1157	0	1095	10	0
2	T	1148	0	1117	3	0
2	U	1159	0	1111	7	0
2	V	1140	0	1111	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1128	0	1078	8	0
2	X	1113	0	1074	5	0
3	A	72	0	61	0	0
3	M	72	0	61	1	0
3	N	72	0	61	1	0
3	P	72	0	61	1	0
4	B	83	0	70	2	0
4	C	83	0	70	0	0
4	Q	83	0	70	1	0
4	R	83	0	70	1	0
5	D	61	0	52	0	0
5	E	61	0	52	2	0
5	F	61	0	52	0	0
5	O	61	0	52	1	0
All	All	32413	0	31385	137	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 2.

The worst 5 of 137 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:J:10:MET:SD	2:J:86:ARG:NH1	2.64	0.71
1:A:159:LEU:O	1:A:160:MET:HG2	1.96	0.65
2:I:55:LEU:HD22	2:I:93:LYS:HD2	1.81	0.63
1:F:159:LEU:O	1:F:160:MET:HG2	1.99	0.62
1:F:23:ALA:CB	1:F:29:VAL:HG21	2.29	0.61

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	184/208 (88%)	177 (96%)	6 (3%)	1 (0%)	32	74
1	B	185/208 (89%)	178 (96%)	7 (4%)	0	100	100
1	C	182/208 (88%)	175 (96%)	6 (3%)	1 (0%)	32	74
1	D	183/208 (88%)	176 (96%)	6 (3%)	1 (0%)	32	74
1	E	183/208 (88%)	176 (96%)	6 (3%)	1 (0%)	32	74
1	F	185/208 (89%)	177 (96%)	7 (4%)	1 (0%)	32	74
1	M	187/208 (90%)	178 (95%)	9 (5%)	0	100	100
1	N	187/208 (90%)	179 (96%)	6 (3%)	2 (1%)	17	60
1	O	182/208 (88%)	176 (97%)	5 (3%)	1 (0%)	32	74
1	P	185/208 (89%)	178 (96%)	6 (3%)	1 (0%)	32	74
1	Q	181/208 (87%)	174 (96%)	6 (3%)	1 (1%)	28	71
1	R	182/208 (88%)	175 (96%)	6 (3%)	1 (0%)	32	74
2	G	143/153 (94%)	139 (97%)	4 (3%)	0	100	100
2	H	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	I	133/153 (87%)	130 (98%)	3 (2%)	0	100	100
2	J	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	K	141/153 (92%)	139 (99%)	2 (1%)	0	100	100
2	L	131/153 (86%)	128 (98%)	3 (2%)	0	100	100
2	S	142/153 (93%)	138 (97%)	4 (3%)	0	100	100
2	T	140/153 (92%)	136 (97%)	4 (3%)	0	100	100
2	U	142/153 (93%)	138 (97%)	4 (3%)	0	100	100
2	V	137/153 (90%)	133 (97%)	4 (3%)	0	100	100
2	W	138/153 (90%)	134 (97%)	4 (3%)	0	100	100
2	X	135/153 (88%)	130 (96%)	5 (4%)	0	100	100
All	All	3868/4332 (89%)	3736 (97%)	121 (3%)	11 (0%)	44	81

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	160	MET
1	A	41	GLY
1	C	41	GLY
1	D	41	GLY
1	E	41	GLY

### 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	166/183 (91%)	166 (100%)	0	100	100
1	B	167/183 (91%)	167 (100%)	0	100	100
1	C	165/183 (90%)	165 (100%)	0	100	100
1	D	166/183 (91%)	166 (100%)	0	100	100
1	E	165/183 (90%)	165 (100%)	0	100	100
1	F	165/183 (90%)	165 (100%)	0	100	100
1	M	166/183 (91%)	166 (100%)	0	100	100
1	N	169/183 (92%)	168 (99%)	1 (1%)	89	94
1	O	164/183 (90%)	164 (100%)	0	100	100
1	P	168/183 (92%)	168 (100%)	0	100	100
1	Q	166/183 (91%)	166 (100%)	0	100	100
1	R	166/183 (91%)	166 (100%)	0	100	100
2	G	133/145 (92%)	132 (99%)	1 (1%)	85	92
2	H	131/145 (90%)	130 (99%)	1 (1%)	85	92
2	I	127/145 (88%)	125 (98%)	2 (2%)	68	85
2	J	132/145 (91%)	131 (99%)	1 (1%)	85	92
2	K	133/145 (92%)	132 (99%)	1 (1%)	85	92
2	L	125/145 (86%)	124 (99%)	1 (1%)	85	92
2	S	132/145 (91%)	131 (99%)	1 (1%)	85	92
2	T	132/145 (91%)	131 (99%)	1 (1%)	85	92
2	U	133/145 (92%)	131 (98%)	2 (2%)	70	86
2	V	131/145 (90%)	130 (99%)	1 (1%)	85	92
2	W	128/145 (88%)	126 (98%)	2 (2%)	68	85
2	X	128/145 (88%)	127 (99%)	1 (1%)	85	92
All	All	3558/3936 (90%)	3542 (100%)	16 (0%)	93	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	172	ASN
2	S	30	SER
2	V	30	SER
2	L	30	SER
2	W	30	SER

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

Mol	Chain	Res	Type
2	K	58	GLN
2	W	70	ASN
1	M	81	HIS
2	G	9	HIS
2	V	42	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

72 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	300	1,3	14,14,15	0.52	0	15,19,21	1.09	1 (6%)
3	NAG	A	301	3	14,14,15	0.53	0	15,19,21	0.69	0
3	BMA	A	302	3	11,11,12	0.67	0	13,15,17	1.00	0
3	MAN	A	303	3	11,11,12	0.56	0	13,15,17	0.96	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MAN	A	304	3	11,11,12	0.59	0	13,15,17	0.82	0
3	MAN	A	305	3	11,11,12	0.60	0	13,15,17	0.76	1 (7%)
4	NAG	B	300	1,4	14,14,15	0.59	0	15,19,21	1.35	3 (20%)
4	NAG	B	301	4	14,14,15	0.53	0	15,19,21	1.00	1 (6%)
4	BMA	B	302	4	11,11,12	0.62	0	13,15,17	2.40	3 (23%)
4	MAN	B	303	4	11,11,12	0.52	0	13,15,17	1.71	2 (15%)
4	MAN	B	304	4	11,11,12	0.58	0	13,15,17	0.63	0
4	MAN	B	305	4	11,11,12	0.59	0	13,15,17	0.78	0
4	MAN	B	306	4	11,11,12	0.65	0	13,15,17	1.58	2 (15%)
4	NAG	C	300	1,4	14,14,15	0.51	0	15,19,21	1.68	2 (13%)
4	NAG	C	301	4	14,14,15	0.55	0	15,19,21	0.99	0
4	BMA	C	302	4	11,11,12	0.56	0	13,15,17	1.92	3 (23%)
4	MAN	C	303	4	11,11,12	0.58	0	13,15,17	1.50	2 (15%)
4	MAN	C	304	4	11,11,12	0.59	0	13,15,17	0.70	0
4	MAN	C	305	4	11,11,12	0.55	0	13,15,17	0.70	0
4	MAN	C	306	4	11,11,12	0.63	0	13,15,17	0.79	1 (7%)
5	NAG	D	300	1,5	14,14,15	0.59	0	15,19,21	1.88	4 (26%)
5	NAG	D	301	5	14,14,15	0.59	0	15,19,21	1.06	1 (6%)
5	BMA	D	302	5	11,11,12	0.58	0	13,15,17	1.55	2 (15%)
5	MAN	D	303	5	11,11,12	0.52	0	13,15,17	0.50	0
5	MAN	D	304	5	11,11,12	0.63	0	13,15,17	0.86	1 (7%)
5	NAG	E	300	1,5	14,14,15	0.65	0	15,19,21	1.20	1 (6%)
5	NAG	E	301	5	14,14,15	0.59	0	15,19,21	0.95	0
5	BMA	E	302	5	11,11,12	0.72	0	13,15,17	1.92	3 (23%)
5	MAN	E	303	5	11,11,12	0.58	0	13,15,17	0.74	0
5	MAN	E	304	5	11,11,12	0.49	0	13,15,17	1.23	2 (15%)
5	NAG	F	300	1,5	14,14,15	0.56	0	15,19,21	1.49	3 (20%)
5	NAG	F	301	5	14,14,15	0.53	0	15,19,21	0.95	1 (6%)
5	BMA	F	302	5	11,11,12	0.78	0	13,15,17	1.46	1 (7%)
5	MAN	F	303	5	11,11,12	0.58	0	13,15,17	0.81	0
5	MAN	F	304	5	11,11,12	0.53	0	13,15,17	1.10	2 (15%)
3	NAG	M	300	1,3	14,14,15	0.55	0	15,19,21	0.92	1 (6%)
3	NAG	M	301	3	14,14,15	0.53	0	15,19,21	0.66	0
3	BMA	M	302	3	11,11,12	0.70	0	13,15,17	0.79	0
3	MAN	M	303	3	11,11,12	0.54	0	13,15,17	1.40	2 (15%)
3	MAN	M	304	3	11,11,12	0.67	0	13,15,17	0.63	0
3	MAN	M	305	3	11,11,12	0.59	0	13,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	300	1,3	14,14,15	0.59	0	15,19,21	1.47	3 (20%)
3	NAG	N	301	3	14,14,15	0.57	0	15,19,21	0.76	0
3	BMA	N	302	3	11,11,12	0.71	0	13,15,17	1.55	2 (15%)
3	MAN	N	303	3	11,11,12	0.49	0	13,15,17	1.50	2 (15%)
3	MAN	N	304	3	11,11,12	0.50	0	13,15,17	1.29	1 (7%)
3	MAN	N	305	3	11,11,12	0.49	0	13,15,17	0.98	1 (7%)
5	NAG	O	300	1,5	14,14,15	0.60	0	15,19,21	1.06	1 (6%)
5	NAG	O	301	5	14,14,15	0.54	0	15,19,21	0.84	0
5	BMA	O	302	5	11,11,12	0.57	0	13,15,17	1.77	3 (23%)
5	MAN	O	303	5	11,11,12	0.55	0	13,15,17	1.04	1 (7%)
5	MAN	O	304	5	11,11,12	0.57	0	13,15,17	0.96	1 (7%)
3	NAG	P	300	1,3	14,14,15	0.55	0	15,19,21	1.17	1 (6%)
3	NAG	P	301	3	14,14,15	0.58	0	15,19,21	1.18	1 (6%)
3	BMA	P	302	3	11,11,12	0.82	0	13,15,17	1.23	1 (7%)
3	MAN	P	303	3	11,11,12	0.61	0	13,15,17	0.55	0
3	MAN	P	304	3	11,11,12	0.64	0	13,15,17	0.64	0
3	MAN	P	305	3	11,11,12	0.65	0	13,15,17	1.03	1 (7%)
4	NAG	Q	300	1,4	14,14,15	0.53	0	15,19,21	1.40	3 (20%)
4	NAG	Q	301	4	14,14,15	0.51	0	15,19,21	0.69	0
4	BMA	Q	302	4	11,11,12	0.75	0	13,15,17	1.28	2 (15%)
4	MAN	Q	303	4	11,11,12	0.60	0	13,15,17	1.64	2 (15%)
4	MAN	Q	304	4	11,11,12	0.59	0	13,15,17	0.80	1 (7%)
4	MAN	Q	305	4	11,11,12	0.51	0	13,15,17	1.35	2 (15%)
4	MAN	Q	306	4	11,11,12	0.60	0	13,15,17	1.16	1 (7%)
4	NAG	R	300	1,4	14,14,15	0.51	0	15,19,21	1.32	1 (6%)
4	NAG	R	301	4	14,14,15	0.58	0	15,19,21	0.75	0
4	BMA	R	302	4	11,11,12	0.70	0	13,15,17	1.70	4 (30%)
4	MAN	R	303	4	11,11,12	0.62	0	13,15,17	1.20	1 (7%)
4	MAN	R	304	4	11,11,12	0.57	0	13,15,17	0.94	1 (7%)
4	MAN	R	305	4	11,11,12	0.64	0	13,15,17	0.61	0
4	MAN	R	306	4	11,11,12	0.47	0	13,15,17	2.14	3 (23%)

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	MAN	A	303	3	-	0/2/19/22	0/1/1/1
3	MAN	A	304	3	-	0/2/19/22	0/1/1/1
3	MAN	A	305	3	-	0/2/19/22	0/1/1/1
4	NAG	B	300	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	301	4	-	0/6/23/26	0/1/1/1
4	BMA	B	302	4	-	0/2/19/22	0/1/1/1
4	MAN	B	303	4	-	0/2/19/22	0/1/1/1
4	MAN	B	304	4	-	0/2/19/22	0/1/1/1
4	MAN	B	305	4	-	0/2/19/22	0/1/1/1
4	MAN	B	306	4	-	0/2/19/22	0/1/1/1
4	NAG	C	300	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	301	4	-	0/6/23/26	0/1/1/1
4	BMA	C	302	4	-	0/2/19/22	0/1/1/1
4	MAN	C	303	4	-	0/2/19/22	0/1/1/1
4	MAN	C	304	4	-	0/2/19/22	0/1/1/1
4	MAN	C	305	4	-	0/2/19/22	0/1/1/1
4	MAN	C	306	4	-	0/2/19/22	0/1/1/1
5	NAG	D	300	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	301	5	-	0/6/23/26	0/1/1/1
5	BMA	D	302	5	-	0/2/19/22	0/1/1/1
5	MAN	D	303	5	-	0/2/19/22	0/1/1/1
5	MAN	D	304	5	-	0/2/19/22	0/1/1/1
5	NAG	E	300	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	301	5	-	0/6/23/26	0/1/1/1
5	BMA	E	302	5	-	0/2/19/22	0/1/1/1
5	MAN	E	303	5	-	0/2/19/22	0/1/1/1
5	MAN	E	304	5	-	0/2/19/22	0/1/1/1
5	NAG	F	300	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	301	5	-	0/6/23/26	0/1/1/1
5	BMA	F	302	5	-	0/2/19/22	0/1/1/1
5	MAN	F	303	5	-	0/2/19/22	0/1/1/1
5	MAN	F	304	5	-	0/2/19/22	0/1/1/1
3	NAG	M	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	301	3	-	0/6/23/26	0/1/1/1
3	BMA	M	302	3	-	0/2/19/22	0/1/1/1
3	MAN	M	303	3	-	0/2/19/22	0/1/1/1
3	MAN	M	304	3	-	0/2/19/22	0/1/1/1
3	MAN	M	305	3	-	0/2/19/22	0/1/1/1
3	NAG	N	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	301	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	N	302	3	-	0/2/19/22	0/1/1/1
3	MAN	N	303	3	-	0/2/19/22	0/1/1/1
3	MAN	N	304	3	-	0/2/19/22	0/1/1/1
3	MAN	N	305	3	-	0/2/19/22	0/1/1/1
5	NAG	O	300	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	301	5	-	0/6/23/26	0/1/1/1
5	BMA	O	302	5	-	0/2/19/22	0/1/1/1
5	MAN	O	303	5	-	0/2/19/22	0/1/1/1
5	MAN	O	304	5	-	0/2/19/22	0/1/1/1
3	NAG	P	300	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	301	3	-	0/6/23/26	0/1/1/1
3	BMA	P	302	3	-	0/2/19/22	0/1/1/1
3	MAN	P	303	3	-	0/2/19/22	0/1/1/1
3	MAN	P	304	3	-	0/2/19/22	0/1/1/1
3	MAN	P	305	3	-	0/2/19/22	0/1/1/1
4	NAG	Q	300	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Q	301	4	-	0/6/23/26	0/1/1/1
4	BMA	Q	302	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	303	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	304	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	305	4	-	0/2/19/22	0/1/1/1
4	MAN	Q	306	4	-	0/2/19/22	0/1/1/1
4	NAG	R	300	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	301	4	-	0/6/23/26	0/1/1/1
4	BMA	R	302	4	-	0/2/19/22	0/1/1/1
4	MAN	R	303	4	-	0/2/19/22	0/1/1/1
4	MAN	R	304	4	-	0/2/19/22	0/1/1/1
4	MAN	R	305	4	-	0/2/19/22	0/1/1/1
4	MAN	R	306	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	300	NAG	O5-C1-C2	-4.75	104.86	111.47
4	C	300	NAG	O5-C1-C2	-4.32	105.46	111.47
4	B	306	MAN	O5-C1-C2	-3.84	104.77	110.79
4	R	300	NAG	O5-C1-C2	-3.64	106.41	111.47
5	E	300	NAG	O5-C1-C2	-3.37	106.78	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	300	NAG	O7-C7-N2-C2

There are no ring outliers.

14 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	300	NAG	1	0
4	B	301	NAG	1	0
4	B	302	BMA	1	0
4	B	306	MAN	1	0
5	E	301	NAG	1	0
5	E	302	BMA	1	0
5	E	304	MAN	1	0
3	M	302	BMA	1	0
3	M	303	MAN	1	0
3	N	300	NAG	1	0
5	O	300	NAG	1	0
3	P	300	NAG	1	0
4	Q	300	NAG	1	0
4	R	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, 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	188/208 (90%)	0.27	1 (0%) 90 86	143, 190, 239, 281	0
1	B	189/208 (90%)	0.34	5 (2%) 56 47	146, 194, 242, 283	0
1	C	186/208 (89%)	0.55	19 (10%) 7 8	157, 209, 248, 289	0
1	D	187/208 (89%)	0.20	4 (2%) 64 56	150, 202, 238, 288	0
1	E	187/208 (89%)	0.63	25 (13%) 4 5	167, 212, 249, 290	0
1	F	189/208 (90%)	0.22	6 (3%) 48 39	145, 205, 246, 291	0
1	M	191/208 (91%)	0.19	1 (0%) 90 86	143, 193, 248, 317	0
1	N	191/208 (91%)	0.32	3 (1%) 72 64	142, 189, 242, 289	0
1	O	186/208 (89%)	0.13	0 100 100	132, 196, 237, 280	0
1	P	189/208 (90%)	0.23	2 (1%) 80 73	153, 193, 245, 281	0
1	Q	185/208 (88%)	0.28	5 (2%) 55 46	146, 199, 240, 280	0
1	R	186/208 (89%)	0.09	1 (0%) 90 86	135, 192, 238, 285	0
2	G	145/153 (94%)	0.37	1 (0%) 87 82	140, 215, 266, 338	0
2	H	142/153 (92%)	0.12	1 (0%) 87 82	155, 230, 283, 323	0
2	I	137/153 (89%)	0.50	12 (8%) 11 10	178, 246, 290, 316	0
2	J	142/153 (92%)	0.27	6 (4%) 37 30	184, 250, 298, 334	0
2	K	143/153 (93%)	0.30	17 (11%) 5 7	179, 248, 296, 336	0
2	L	135/153 (88%)	0.92	25 (18%) 1 3	187, 248, 301, 350	0
2	S	144/153 (94%)	0.16	0 100 100	161, 225, 278, 327	0
2	T	142/153 (92%)	0.11	3 (2%) 64 56	164, 240, 292, 331	0
2	U	144/153 (94%)	-0.02	0 100 100	176, 243, 299, 325	0
2	V	141/153 (92%)	0.24	8 (5%) 24 21	166, 237, 280, 324	0
2	W	142/153 (92%)	0.21	2 (1%) 75 67	169, 235, 288, 321	0
2	X	139/153 (90%)	0.15	2 (1%) 75 67	159, 228, 282, 314	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3950/4332 (91%)	0.28	149 (3%)	41	33	132, 210, 279, 350	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	SER	6.2
2	L	7	CYS	5.0
2	L	44	LYS	5.0
1	C	189	LEU	4.7
2	L	70	ASN	4.4

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	O	300	14/15	0.94	0.35	-0.01	164,202,282,318	0
5	NAG	F	300	14/15	0.92	0.28	-0.24	194,268,287,303	0
3	NAG	A	300	14/15	0.94	0.28	-0.38	158,184,245,246	0
3	NAG	M	300	14/15	0.96	0.31	-0.38	142,190,244,278	0
3	NAG	N	300	14/15	0.93	0.31	-0.41	101,187,221,223	0
4	NAG	R	300	14/15	0.84	0.26	-0.52	154,190,260,269	0
3	NAG	P	300	14/15	0.91	0.27	-0.54	129,218,239,239	0
5	NAG	E	300	14/15	0.85	0.22	-0.59	185,254,298,308	0
4	NAG	C	300	14/15	0.84	0.19	-0.62	223,276,318,345	0
4	NAG	B	300	14/15	0.94	0.24	-0.68	158,192,224,246	0
5	NAG	D	300	14/15	0.92	0.20	-0.84	202,246,270,275	0
4	NAG	Q	300	14/15	0.91	0.22	-1.15	172,210,247,251	0
4	MAN	C	306	11/12	0.82	0.25	-	178,249,271,281	0
4	MAN	R	304	11/12	0.85	0.25	-	233,279,298,326	0
4	MAN	B	304	11/12	0.77	0.30	-	219,268,297,306	0
4	MAN	Q	305	11/12	0.86	0.32	-	254,324,359,371	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	N	301	14/15	0.92	0.30	-	113,159,214,279	0
3	NAG	A	301	14/15	0.94	0.30	-	111,181,227,233	0
4	MAN	B	305	11/12	0.75	0.25	-	227,270,316,333	0
3	MAN	M	305	11/12	0.88	0.22	-	159,266,328,347	0
5	MAN	E	304	11/12	0.76	0.28	-	222,282,306,313	0
5	MAN	F	304	11/12	0.64	0.35	-	223,300,324,344	0
3	MAN	A	304	11/12	0.79	0.31	-	172,278,292,311	0
4	MAN	Q	306	11/12	0.73	0.32	-	200,242,264,268	0
4	MAN	R	306	11/12	0.81	0.22	-	216,284,323,332	0
5	MAN	F	303	11/12	0.87	0.27	-	229,290,322,341	0
4	MAN	Q	303	11/12	0.77	0.19	-	268,299,347,351	0
4	NAG	C	301	14/15	0.84	0.31	-	182,258,282,287	0
3	MAN	M	303	11/12	0.72	0.22	-	242,274,322,327	0
5	NAG	D	301	14/15	0.86	0.24	-	152,204,221,276	0
3	MAN	M	304	11/12	0.66	0.27	-	229,267,300,324	0
3	MAN	A	305	11/12	0.83	0.23	-	179,283,319,340	0
3	MAN	P	303	11/12	0.90	0.28	-	235,283,301,320	0
5	MAN	E	303	11/12	0.73	0.23	-	184,249,291,304	0
4	BMA	Q	302	11/12	0.90	0.16	-	175,205,224,271	0
5	BMA	F	302	11/12	0.80	0.19	-	197,221,242,300	0
4	NAG	R	301	14/15	0.86	0.28	-	171,184,232,241	0
3	NAG	P	301	14/15	0.94	0.25	-	109,185,229,268	0
4	MAN	C	305	11/12	0.68	0.45	-	217,289,309,314	0
4	MAN	C	304	11/12	0.47	0.92	-	240,308,366,376	0
4	MAN	B	303	11/12	0.86	0.24	-	270,298,320,337	0
5	MAN	D	303	11/12	0.64	0.35	-	186,281,322,333	0
4	BMA	C	302	11/12	0.79	0.31	-	208,249,289,300	0
3	MAN	A	303	11/12	0.86	0.26	-	215,291,309,312	0
3	MAN	N	303	11/12	0.83	0.20	-	222,259,293,368	0
3	BMA	M	302	11/12	0.87	0.15	-	199,229,289,318	0
3	MAN	P	304	11/12	0.77	0.35	-	294,320,348,349	0
3	BMA	P	302	11/12	0.83	0.18	-	189,230,277,279	0
5	BMA	O	302	11/12	0.94	0.18	-	202,211,256,269	0
4	MAN	R	303	11/12	0.83	0.14	-	256,287,316,320	0
5	BMA	D	302	11/12	0.89	0.22	-	191,228,274,332	0
5	MAN	D	304	11/12	0.86	0.31	-	204,256,281,283	0
4	BMA	B	302	11/12	0.95	0.12	-	176,222,235,279	0
5	NAG	O	301	14/15	0.94	0.27	-	147,178,203,238	0
3	BMA	N	302	11/12	0.94	0.13	-	122,186,227,233	0
3	BMA	A	302	11/12	0.86	0.14	-	196,227,268,279	0
5	MAN	O	303	11/12	0.91	0.28	-	172,240,270,283	0
4	NAG	B	301	14/15	0.95	0.30	-	145,197,251,263	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	P	305	11/12	0.74	0.29	-	214,290,327,327	0
4	MAN	R	305	11/12	0.51	0.36	-	248,304,355,371	0
5	NAG	F	301	14/15	0.92	0.21	-	154,216,246,271	0
5	MAN	O	304	11/12	0.84	0.27	-	213,249,288,290	0
4	MAN	B	306	11/12	0.89	0.24	-	186,234,277,304	0
4	MAN	Q	304	11/12	0.79	0.20	-	189,286,305,313	0
5	NAG	E	301	14/15	0.90	0.27	-	206,257,279,286	0
3	MAN	N	305	11/12	0.81	0.24	-	183,247,291,293	0
4	MAN	C	303	11/12	0.62	0.51	-	292,310,342,361	0
3	NAG	M	301	14/15	0.93	0.27	-	157,188,237,248	0
3	MAN	N	304	11/12	0.77	0.30	-	165,285,305,311	0
4	BMA	R	302	11/12	0.96	0.12	-	155,209,248,250	0
4	NAG	Q	301	14/15	0.93	0.28	-	148,181,242,292	0
5	BMA	E	302	11/12	0.79	0.12	-	239,257,278,284	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.