



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2020 – 12:07 PM EST

PDB ID : 7KBT
Title : Factor VIII in complex with the anti-C2 domain antibody, G99
Authors : Ronayne, E.K.; Gish, J.; Wilson, C.; Peters, S.; Spencer, H.T.; Spiegel, P.C.; Childers, K.C.
Deposited on : 2020-10-02
Resolution : 4.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

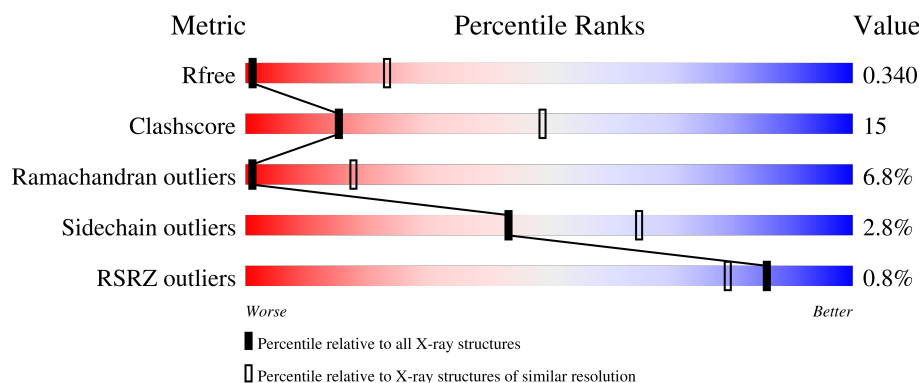
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



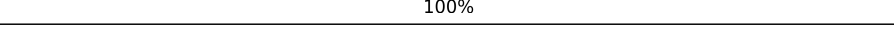
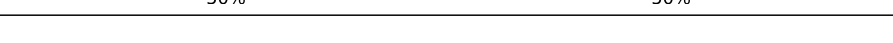
The reported resolution of this entry is 4.15 Å.

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}	130704	1020 (4.54-3.76)
Clashscore	141614	1028 (4.52-3.80)
Ramachandran outliers	138981	1005 (4.54-3.78)
Sidechain outliers	138945	1024 (4.54-3.76)
RSRZ outliers	127900	1055 (4.62-3.70)

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 respectively. 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	1467	
2	E	224	
3	F	214	
4	B	2	
4	G	2	

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
4	NAG	B	2	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11366 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 Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1233	Total	C	N	O	S	0	0	0
			9809	6272	1700	1785	52			

- Molecule 2 is a protein called G99 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	115	Total	C	N	O	S	0	0	0
			818	503	139	173	3			

- Molecule 3 is a protein called G99 light chain.

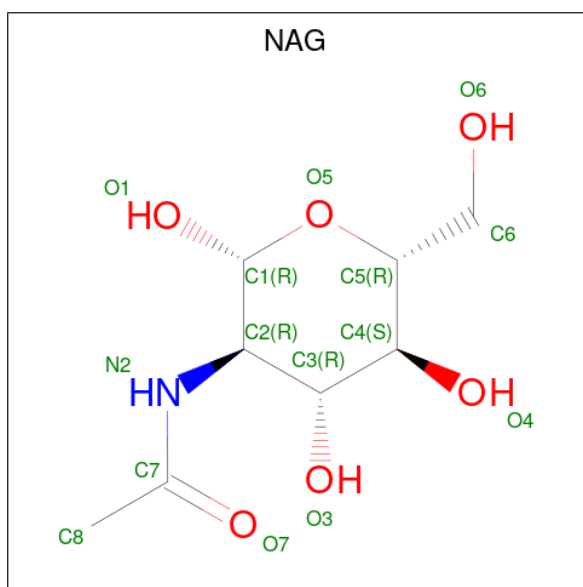
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	96	Total	C	N	O	S	0	0	0
			666	403	120	140	3			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

● Molecule 1: Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII,Coagulation factor VIII

SER	P685	MET	M467	TLE	T999	A212	L130	MET	GLN
ARG	G686	S568	Q468	ARG		ASN	P131	GLN	
PRO	L687	D569	Q468	SER	Q306	ASN	G132	LEU	E54
PRO	w688	K570	P472	VAL		ASP	K133	GLU	D57
SER	t689	R571	Y473	ALA	C311	TRP	SER	LEU	
ALA	L690	M572	M474	LYS	H312	THR	Q135	SER	A63
SER	G691	R583	L486	K377	I313	ARG	T136	THR	R64
ALA	G692	I591	Y487	T381	S314	ALA	Y137	CYS	P65
PRO	H693	I591	S488		S315	MET	W138	PHE	R66
LYS	N694	L595	R489	P397	H318	ASP	W139	LEU	w69
PRO	S695	L595	R490	L398	G319	PRD	Q140	LEU	M70
PRO	D696	L595	R490	L398	G320	ALA	Y141	LEU	G71
VAL	F697	L595	L491	V399	M321	ALA	T148	LEU	L72
LEU	N698	A599	G494	L400	V325	ARG		PRO	L73
ARG	N699	G600	A401	A401	R326	ARG	P153	PRO	G74
ARG	R700	V601	P402	P402	V327	ARG	G154	LEU	P75
HIS		G602	K496	D403	R328	ARG	L155	PHE	T76
GLN	T703	L603	H497	D404	V327	ARG	T156	GLY	I77
GLN	A704	E604	R498	R405	E328	ARG	Y157	SER	
ARG	R705	E604	K499	S406	A331	ARG		ALA	A1
ASP	L706	E607	Y407	Y407	E332	VAL	E80	ALA	R4
ILE	L706	E607	Y407	Y407	E332	VAL	E80	ALA	Y5
SER	K707	S616	P502	K408	GLU	W235	T88	ALA	
LEU	W708	I503	S409	S409	PRD	G237	L89	ALA	G8
PRO	S709	T617	L504		GLN	Y238	K90	VAL	
THR	S710	M618	P505	M413	LEU	W239	N91	GLU	
PHE	C711	G619	G506		LEU			GLU	
ASP	ASP	Y620	ASP	P416	ARG	S242	H95	VAL	
GLN	GLN	V621	T516	Q417	ARG	L243	P96	VAL	
LYS	LYS	F622	V517	R418	LYS		V97	GLU	
ASN	ASN			I419	ALA	L246		GLU	
THR	THR	D693			ALA				
GLY	GLY	S624	P521	K422	ASP	G247			
ASP	ASP	T522	T522		GLU	L247	A101		D15
LYS	LYS	K523	K523		GLU	C249	G102		Y16
MET	MET	L627	S524	R427	GLU	H250	V103		E24
THR	THR	S628	D525		ASP	K251	V104		L25
GLY	GLY	V629	P526		TYR	K252	S105		H26
ASP	ASP	G629		A430	ASP		F105		VAL
ASP	ASP	L631	L529	Y431	ASP	W256	W107		
ILE	ILE	L631	L529	T432	ASP		K108		D28
PHE	PHE	GLU		D433	ASN		K107		R30
GLY	GLY	Y533	Y533	E434	LEU	L259	S109		R30
SER	SER	F648	S534	T435	TYR		S110		PHE
THR	THR	L649	S535	F436	ASP	P265	E111		PRO
GLY	GLY	S650	S535	K437	SER	E266	G112		ALA
ALA	ALA	E540	E540	T438	ASP		A113		THR
LYS	LYS	V651	R541	R439	MET	L270	Y115		ALA
LEU	LEU	S654	D542	E440	ASP		T190		PRO
LEU	LEU	G655			VAL	E273	Q191		GLY
SER	SER	Y656	S545	H444	VAL		M192		ALA
PHE	PHE	Y656	S545	H444	VAL		D117		ALA
ASP	ASP	F657	K556	E445	ARG	W279	H118		LEU
ASN	ASN	F658	K556	E445	ARG	R280	T119		PRO
ASN	ASN	F658	K556	E445	ARG	R280	S120		LEU



SER
THR
TYR
SER
MET
SER
SER
THR
LEU
THR
THR
LEU
THR
LYS
ASP
GLU
TYR
GLU
ARG
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PHE
ASN
ARG
ASN
GLU
CYS

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.24Å 132.24Å 380.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.48 – 4.15 25.72 – 4.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (25.48-4.15) 99.7 (25.72-4.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 4.10Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.300 , 0.338 0.300 , 0.340	Depositor DCC
R_{free} test set	1987 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å ²)	195.9	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 139.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, CA, CU, 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	0.29	0/10070	0.63	3/13647 (0.0%)
2	E	0.26	0/833	0.48	0/1129
3	F	0.25	0/673	0.48	0/906
All	All	0.29	0/11576	0.61	3/15682 (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	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	C-N-CA	6.71	138.46	121.70
1	A	491	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	A	449	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2057	GLY	Peptide
1	A	404	ASP	Peptide
1	A	570	LYS	Peptide
1	A	691	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	696	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	9809	0	9455	310	0
2	E	818	0	700	16	0
3	F	666	0	587	10	0
4	B	28	0	25	0	0
4	G	28	0	25	1	0
5	A	14	0	13	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0
All	All	11366	0	10805	331	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 15.

The worst 5 of 331 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:A:1781:ARG:HG2	1:A:1782:PRO:HD2	1.49	0.93
1:A:540:GLU:HG2	1:A:583:ARG:HH21	1.39	0.85
1:A:64:ARG:HH21	1:A:65:PRO:HD2	1.41	0.85
1:A:1927:ASP:HA	1:A:2012:THR:HA	1.58	0.84
1:A:54:GLU:HG2	1:A:75:PRO:HG3	1.58	0.83

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1211/1467 (82%)	952 (79%)	170 (14%)	89 (7%)	1	16
2	E	105/224 (47%)	82 (78%)	19 (18%)	4 (4%)	3	27
3	F	90/214 (42%)	63 (70%)	24 (27%)	3 (3%)	4	30
All	All	1406/1905 (74%)	1097 (78%)	213 (15%)	96 (7%)	1	18

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	229	GLN
1	A	250	HIS
1	A	265	PRO
1	A	291	PRO

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	1052/1301 (81%)	1026 (98%)	26 (2%)	47	68
2	E	80/191 (42%)	77 (96%)	3 (4%)	33	58
3	F	64/191 (34%)	60 (94%)	4 (6%)	18	45
All	All	1196/1683 (71%)	1163 (97%)	33 (3%)	43	65

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1753	ASN
1	A	2018	SER
3	F	56	SER
1	A	1983	PHE
1	A	1997	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	GLN
1	A	694	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 ⓘ

4 monosaccharides 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	1	1,4	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	B	2	4	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	G	1	1,4	14,14,15	0.70	1 (7%)	17,19,21	0.65	1 (5%)
4	NAG	G	2	4	14,14,15	0.91	1 (7%)	17,19,21	1.24	3 (17%)

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	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	NAG	O5-C1	-2.52	1.39	1.43
4	G	1	NAG	O5-C1	2.28	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C4-C3-C2	2.72	115.00	111.02
4	G	2	NAG	C2-N2-C7	2.46	126.41	122.90
4	G	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	G	2	NAG	C3-C4-C5	2.01	113.83	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	2	NAG	C1

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C4-C5-C6-O6
4	B	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
5	NAG	A	2401	1	14,14,15	0.30	0	17,19,21	0.50	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
5	NAG	A	2401	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2401	NAG	C4-C5-C6-O6
5	A	2401	NAG	O5-C5-C6-O6
5	A	2401	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1233/1467 (84%)	-0.28	7 (0%) 89 84	194, 241, 289, 329	0
2	E	115/224 (51%)	-0.01	1 (0%) 84 77	265, 306, 326, 335	0
3	F	96/214 (44%)	0.17	3 (3%) 49 38	277, 329, 358, 365	0
All	All	1444/1905 (75%)	-0.23	11 (0%) 86 79	194, 247, 324, 365	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	14	SER	2.8
3	F	82	ASP	2.7
1	A	2201	ALA	2.6
1	A	89	LEU	2.5
1	A	556	LYS	2.4

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. 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	B-factors(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.69	0.38	224,248,256,258	0
4	NAG	B	2	14/15	0.81	0.40	301,312,318,318	0
4	NAG	G	1	14/15	0.81	0.43	243,253,266,267	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	1	14/15	0.88	0.35	261,277,285,288	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. 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	B-factors(\AA^2)	Q<0.9
6	CU	A	2402	1/1	0.83	0.16	229,229,229,229	0
5	NAG	A	2401	14/15	0.87	0.23	273,291,300,302	0
7	ZN	A	2403	1/1	0.90	0.19	213,213,213,213	0
8	CA	A	2404	1/1	0.97	0.22	210,210,210,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.