

wwPDB X-ray Structure Validation Summary Report (i)

Jan 16, 2024 - 04:03 PM EST

PDB ID	:	8TW3
Title	:	hMPV fusion protein complexed with single domain antibodies sdHMPV16
		and sdHMPV12
Authors	:	Rush, S.A.; McLellan, J.S.
Deposited on	:	2023-08-19
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.90 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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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 <=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	٨	109							
	A	193	61%	•	36%				
1	v	102	610/		2.64				
	1	195	61%	•	36%				
2	В	192	58%	6% •	36%				
			% •						
2	Z	192	54%	8%	38%				
		- 10	.% ■	_	_				
3	F,	542	68%		28%				



Mol	Chain	Length	Quality	of chain	
			.% ■		
3	Х	542	61%	8%	31%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18851 atoms, of which 9276 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 Single domain antibody sdHMPV12.

Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
1	А	123	Total	С	Η	Ν	0	S	0	0	0
-		120	1813	568	894	164	182	5	0	Ŭ	Ŭ
1	v	192	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
L	I	123	1813	568	894	164	182	5	0	0	0

• Molecule 2 is a protein called Single domain antibody sdHMPV16.

Mol	Chain	Residues			Aton	ns			ZeroOcc	AltConf	Trace
0	Р	192	Total	С	Η	Ν	0	S	0	0	0
	D	123	1826	580	883	170	188	5	0	0	0
0	7	110	Total	С	Н	Ν	0	S	0	0	0
		119	1774	570	851	166	182	5		U	0

• Molecule 3 is a protein called Fusion glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	F	388	Total 5018	C 1844	H 2066	N 510	0 577	S 21	0	0	0
			- 5918 	1844	2900	310	011	21			
3	3 X	376	Total	С	Н	Ν	O	\mathbf{S}	0	0	0
J A	510	5599	1792	2736	494	556	21		U		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	185	PRO	ALA	conflict	UNP H6X1Z0
F	491	GLY	-	expression tag	UNP H6X1Z0
F	492	GLY	-	expression tag	UNP H6X1Z0
F	493	GLY	-	expression tag	UNP H6X1Z0
F	494	SER	-	expression tag	UNP H6X1Z0
F	495	LEU	-	expression tag	UNP H6X1Z0
F	496	GLU	-	expression tag	UNP H6X1Z0
F	497	VAL	_	expression tag	UNP H6X1Z0



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Chain	Residue	Modelled	Actual	Comment	Reference
F	498	LEU	-	expression tag	UNP H6X1Z0
F	499	PHE	-	expression tag	UNP H6X1Z0
F	500	GLN	-	expression tag	UNP H6X1Z0
F	501	GLY	-	expression tag	UNP H6X1Z0
F	502	PRO	-	expression tag	UNP H6X1Z0
F	503	GLY	-	expression tag	UNP H6X1Z0
F	504	HIS	-	expression tag	UNP H6X1Z0
F	505	HIS	-	expression tag	UNP H6X1Z0
F	506	HIS	-	expression tag	UNP H6X1Z0
F	507	HIS	-	expression tag	UNP H6X1Z0
F	508	HIS	-	expression tag	UNP H6X1Z0
F	509	HIS	-	expression tag	UNP H6X1Z0
F	510	HIS	-	expression tag	UNP H6X1Z0
F	511	HIS	-	expression tag	UNP H6X1Z0
F	512	SER	-	expression tag	UNP H6X1Z0
F	513	ALA	-	expression tag	UNP H6X1Z0
F	514	TRP	-	expression tag	UNP H6X1Z0
F	515	SER	-	expression tag	UNP H6X1Z0
F	516	HIS	-	expression tag	UNP H6X1Z0
F	517	PRO	-	expression tag	UNP H6X1Z0
F	518	GLN	-	expression tag	UNP H6X1Z0
F	519	PHE	-	expression tag	UNP H6X1Z0
F	520	GLU	-	expression tag	UNP H6X1Z0
F	521	LYS	-	expression tag	UNP H6X1Z0
F	522	GLY	-	expression tag	UNP H6X1Z0
F	523	GLY	-	expression tag	UNP H6X1Z0
F	524	GLY	-	expression tag	UNP H6X1Z0
F	525	SER	-	expression tag	UNP H6X1Z0
F	526	GLY	-	expression tag	UNP H6X1Z0
F	527	GLY	-	expression tag	UNP H6X1Z0
F	528	GLY	-	expression tag	UNP H6X1Z0
F	529	GLY	-	expression tag	UNP H6X1Z0
F	530	SER	-	expression tag	UNP H6X1Z0
F	531	GLY	-	expression tag	UNP H6X1Z0
F	532	GLY	-	expression tag	UNP H6X1Z0
F	533	SER	-	expression tag	UNP H6X1Z0
F	534	ALA	-	expression tag	UNP H6X1Z0
F	535	TRP	-	expression tag	UNP H6X1Z0
F	536	SER	-	expression tag	UNP H6X1Z0
F	537	HIS	-	expression tag	UNP H6X1Z0
F	538	PRO	-	expression tag	UNP H6X1Z0
F	539	GLN	-	expression tag	UNP H6X1Z0



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Chain	Residue	Modelled	Actual	Comment	Reference
F	540	PHE	-	expression tag	UNP H6X1Z0
F	541	GLU	-	expression tag	UNP H6X1Z0
F	542	LYS	-	expression tag	UNP H6X1Z0
Х	185	PRO	ALA	conflict	UNP H6X1Z0
Х	491	GLY	-	expression tag	UNP H6X1Z0
Х	492	GLY	-	expression tag	UNP H6X1Z0
Х	493	GLY	-	expression tag	UNP H6X1Z0
Х	494	SER	-	expression tag	UNP H6X1Z0
Х	495	LEU	-	expression tag	UNP H6X1Z0
Х	496	GLU	-	expression tag	UNP H6X1Z0
Х	497	VAL	-	expression tag	UNP H6X1Z0
Х	498	LEU	-	expression tag	UNP H6X1Z0
Х	499	PHE	-	expression tag	UNP H6X1Z0
Х	500	GLN	-	expression tag	UNP H6X1Z0
Х	501	GLY	-	expression tag	UNP H6X1Z0
Х	502	PRO	-	expression tag	UNP H6X1Z0
Х	503	GLY	-	expression tag	UNP H6X1Z0
Х	504	HIS	-	expression tag	UNP H6X1Z0
Х	505	HIS	-	expression tag	UNP H6X1Z0
Х	506	HIS	-	expression tag	UNP H6X1Z0
Х	507	HIS	-	expression tag	UNP H6X1Z0
Х	508	HIS	-	expression tag	UNP H6X1Z0
Х	509	HIS	-	expression tag	UNP H6X1Z0
Х	510	HIS	-	expression tag	UNP H6X1Z0
Х	511	HIS	-	expression tag	UNP H6X1Z0
Х	512	SER	-	expression tag	UNP H6X1Z0
Х	513	ALA	-	expression tag	UNP H6X1Z0
Х	514	TRP	-	expression tag	UNP H6X1Z0
Х	515	SER	-	expression tag	UNP H6X1Z0
Х	516	HIS	-	expression tag	UNP H6X1Z0
Х	517	PRO	-	expression tag	UNP H6X1Z0
Х	518	GLN	-	expression tag	UNP H6X1Z0
Х	519	PHE	-	expression tag	UNP H6X1Z0
Х	520	GLU	-	expression tag	UNP H6X1Z0
Х	521	LYS	-	expression tag	UNP H6X1Z0
Х	522	GLY	-	expression tag	UNP H6X1Z0
Х	523	GLY	-	expression tag	UNP H6X1Z0
Х	524	GLY	-	expression tag	UNP H6X1Z0
Х	525	SER	-	expression tag	UNP H6X1Z0
Х	526	GLY	-	expression tag	UNP H6X1Z0
Х	527	GLY	-	expression tag	UNP H6X1Z0
Х	528	GLY	-	expression tag	UNP H6X1Z0



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Chain	Residue	Modelled	Actual	Comment	Reference
Х	529	GLY	-	expression tag	UNP H6X1Z0
Х	530	SER	-	expression tag	UNP H6X1Z0
Х	531	GLY	-	expression tag	UNP H6X1Z0
Х	532	GLY	-	expression tag	UNP H6X1Z0
X	533	SER	-	expression tag	UNP H6X1Z0
X	534	ALA	-	expression tag	UNP H6X1Z0
X	535	TRP	-	expression tag	UNP H6X1Z0
X	536	SER	-	expression tag	UNP H6X1Z0
X	537	HIS	-	expression tag	UNP H6X1Z0
Х	538	PRO	-	expression tag	UNP H6X1Z0
X	539	GLN	-	expression tag	UNP H6X1Z0
X	540	PHE	-	expression tag	UNP H6X1Z0
X	541	GLU	-	expression tag	UNP H6X1Z0
X	542	LYS	-	expression tag	UNP H6X1Z0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	
4	Г	1	Total	С	Η	Ν	Ο	0	0	
4	Г	1	27	8	13	1	5	0		
4	F	1	1 Total C H N O		0	0				
4	Г	1	27	8	13	1	5	0	0	
4	v	1	Total	С	Η	Ν	Ο	0	0	
4		1	27	8	13	1	5	0	0	
4	v	1	Total	С	Η	Ν	0	0	0	
4	Λ		27	8	13	1	5		0	



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Single domain antibody sdHMPV12









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	80.26Å 115.61Å 158.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	44.97 - 2.90	Depositor
	44.97 - 2.90	EDS
% Data completeness	97.9 (44.97-2.90)	Depositor
(in resolution range)	97.9(44.97-2.90)	EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.10 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
P. P.	0.191 , 0.232	Depositor
n, n_{free}	0.205 , 0.243	DCC
R_{free} test set	1541 reflections (4.72%)	wwPDB-VP
Wilson B-factor $(Å^2)$	41.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 38.6	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18851	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 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).

Mal	Chain	Bond	lengths	Bond angles		
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/936	0.53	0/1271	
1	Y	0.28	0/936	0.53	0/1271	
2	В	0.28	0/962	0.54	0/1302	
2	Ζ	0.27	0/941	0.52	0/1273	
3	F	0.26	0/2991	0.50	0/4052	
3	Х	0.27	0/2902	0.51	0/3931	
All	All	0.27	0/9668	0.51	0/13100	

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	А	919	894	896	3	0
1	Y	919	894	896	3	0
2	В	943	883	890	10	0
2	Ζ	923	851	873	8	0
3	F	2952	2966	2973	10	0
3	Х	2863	2736	2889	26	0
4	F	28	26	26	1	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Х	28	26	26	2	0
All	All	9575	9276	9469	58	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 3.

The worst 5 of 58 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)	
3:X:287:LYS:NZ	3:X:323:GLU:OE2	2.00	0.94	
3:X:184:ILE:HG22	3:X:186:ASP:H	1.47	0.80	
2:Z:97:GLU:N	2:Z:97:GLU:OE1	2.18	0.76	
3:F:87:ASP:OD1	3:X:126:LYS:NZ	2.27	0.66	
3:X:353:ASN:HD21	4:X:601:NAG:C1	2.08	0.66	

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	Perce	ntiles
1	А	121/193~(63%)	117 (97%)	4 (3%)	0	100	100
1	Y	121/193~(63%)	117 (97%)	4 (3%)	0	100	100
2	В	121/192~(63%)	118 (98%)	3 (2%)	0	100	100
2	Z	115/192~(60%)	110 (96%)	5 (4%)	0	100	100
3	F	384/542~(71%)	374 (97%)	10 (3%)	0	100	100
3	Х	372/542~(69%)	357~(96%)	15 (4%)	0	100	100
All	All	1234/1854~(67%)	1193 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.



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	А	99/151~(66%)	99~(100%)	0	100	100	
1	Y	99/151~(66%)	98~(99%)	1 (1%)	76	92	
2	В	98/149~(66%)	97~(99%)	1 (1%)	76	92	
2	Ζ	96/149~(64%)	96 (100%)	0	100	100	
3	F	329/453~(73%)	325~(99%)	4 (1%)	71	91	
3	Х	320/453~(71%)	317 (99%)	3 (1%)	78	93	
All	All	1041/1506~(69%)	1032 (99%)	9 (1%)	78	93	

 $5~{\rm of}~9$ residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
3	Х	193	PHE
1	Y	92	ASN
3	F	193	PHE
3	F	272	GLN
3	Х	163	ARG

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

Mol	Chain	Res	Type
2	В	90	GLN
3	Х	353	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mal	Mol Type Chain		Dog	Pog Link	Bond lengths			Bond angles		
	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	602	3	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	Х	602	3	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	Х	601	-	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	F	601	-	14,14,15	0.23	0	17,19,21	0.46	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
4	NAG	F	602	3	-	2/6/23/26	0/1/1/1
4	NAG	Х	602	3	-	0/6/23/26	0/1/1/1
4	NAG	Х	601	-	-	0/6/23/26	0/1/1/1
4	NAG	F	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	602	NAG	O5-C5-C6-O6
4	F	602	NAG	C4-C5-C6-O6



There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	602	NAG	1	0
4	Х	601	NAG	2	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 (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, 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	А	123/193~(63%)	-0.01	0 100 100	19, 32, 48, 65	0
1	Y	123/193~(63%)	-0.03	0 100 100	20, 32, 52, 62	0
2	В	123/192~(64%)	0.25	0 100 100	23, 49, 79, 115	0
2	Z	119/192~(61%)	0.45	2 (1%) 70 69	32, 60, 84, 94	0
3	F	388/542~(71%)	0.18	5 (1%) 77 77	19, 39, 72, 107	0
3	Х	376/542~(69%)	0.13	5 (1%) 77 77	16, 41, 79, 90	0
All	All	1252/1854~(67%)	0.16	12 (0%) 82 82	16, 40, 78, 115	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Х	296	LYS	4.4
2	Ζ	83	ALA	3.4
3	F	296	LYS	3.3
3	F	144	THR	3.0
2	Ζ	1	GLN	2.6

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)

There are no monosaccharides in this entry.



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, 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	NAG	Х	601	14/15	0.75	0.37	53,88,110,113	0
4	NAG	F	601	14/15	0.84	0.27	$60,\!78,\!101,\!115$	0
4	NAG	Х	602	14/15	0.89	0.25	54,64,76,77	0
4	NAG	F	602	14/15	0.90	0.22	53,64,73,78	0

6.5 Other polymers (i)

There are no such residues in this entry.

