



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2019 – 10:05 AM EDT

PDB ID : 2QAD  
Title : Structure of tyrosine-sulfated 412d antibody complexed with HIV-1 YU2 gp120 and CD4  
Authors : Huang, C.-C.; Tang, M.; Robinson, J.; Wyatt, R.; Kwong, P.D.  
Deposited on : 2007-06-14  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

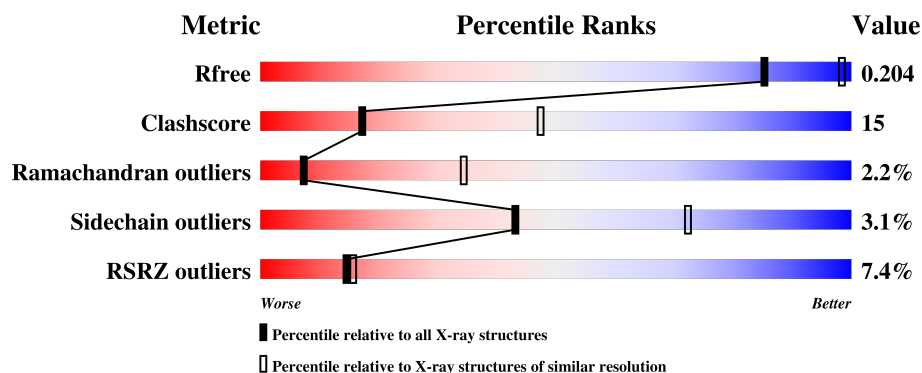
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	111664	1168 (3.36-3.24)
Clashscore	122126	1022 (3.34-3.26)
Ramachandran outliers	120053	1004 (3.34-3.26)
Sidechain outliers	120020	1003 (3.34-3.26)
RSRZ outliers	108989	1133 (3.36-3.24)

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	322	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>33%</div> <div>..</div> </div> </div>
1	E	322	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>..</div> </div> </div>
2	B	181	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>..</div> </div> </div>
2	F	181	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>..</div> </div> </div>
3	C	214	<div> <div>12%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	214	
4	D	231	
4	H	231	

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
5	NAG	A	856	-	-	-	X
5	NAG	A	862	X	-	-	X
5	NAG	A	894	X	-	-	X
5	NAG	A	900	-	-	-	X
5	NAG	A	963	-	-	-	X
5	NAG	E	856	-	-	-	X
5	NAG	E	862	X	-	-	X
5	NAG	E	894	-	-	-	X
5	NAG	E	963	X	-	-	X
6	MLA	A	3	-	-	-	X
7	EDO	C	216	-	-	-	X
7	EDO	F	187	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14987 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2499	1562	445	474	18			
1	E	312	Total	C	N	O	S	0	0	0
			2445	1533	430	464	18			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1383	865	242	272	4			
2	F	179	Total	C	N	O	S	0	0	0
			1394	874	243	273	4			

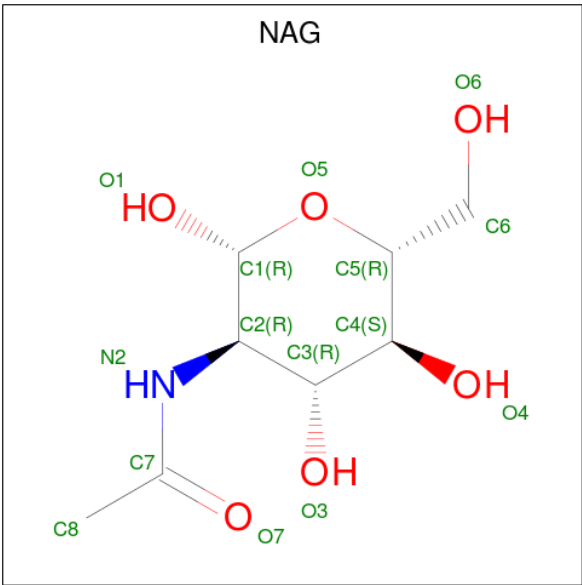
- Molecule 3 is a protein called anti-HIV-1 antibody 412d light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			
3	G	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			

- Molecule 4 is a protein called anti-HIV-1 antibody 412d heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			
4	H	231	Total	C	N	O	S	0	0	0
			1746	1101	286	350	9			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



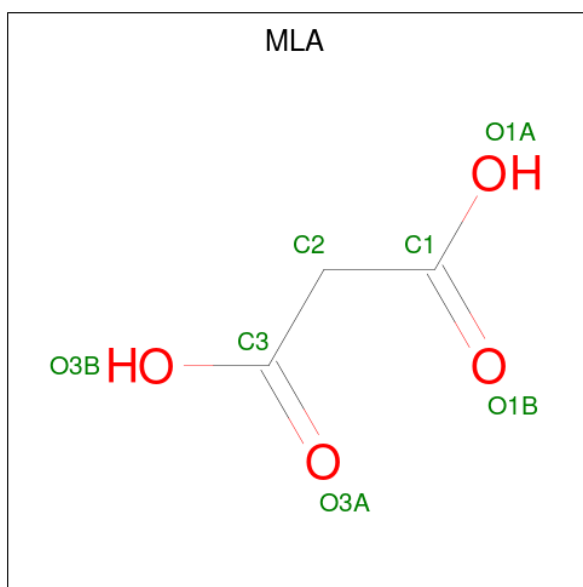
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

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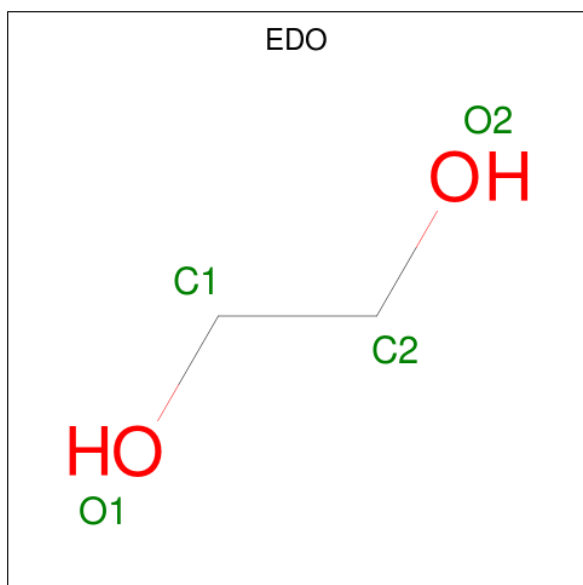
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1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

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	B	1	Total	C	O	0	0
			7	3	4		
6	F	1	Total	C	O	0	0
			7	3	4		
6	H	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



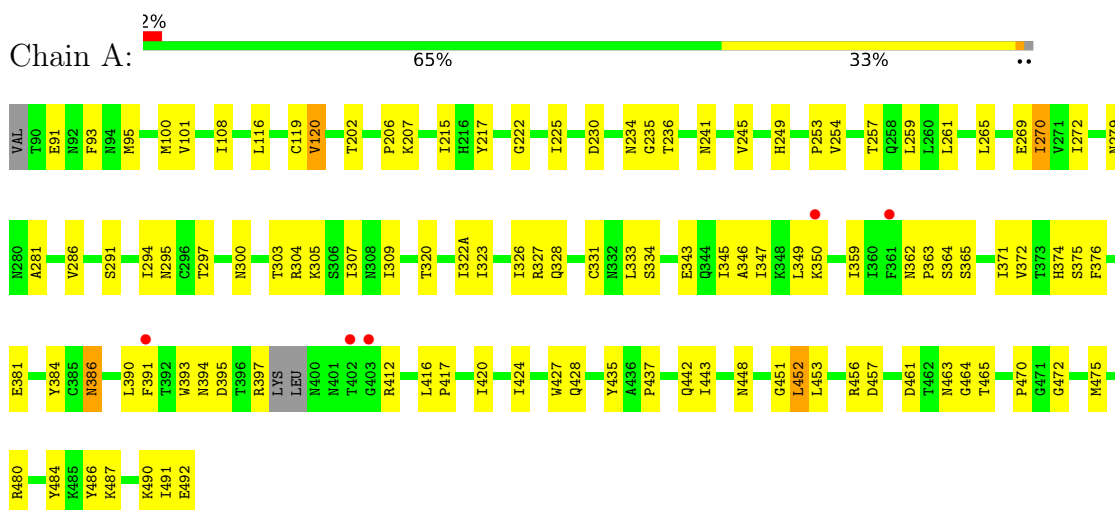
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	C	1	Total 4	C 2	O 2	0	0
7	D	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	F	1	Total 4	C 2	O 2	0	0



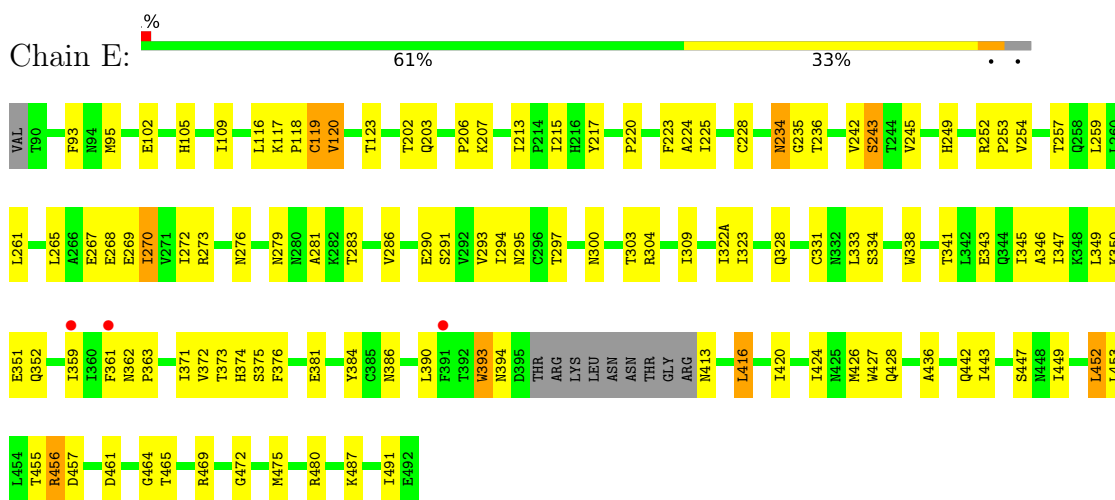
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Envelope glycoprotein gp160

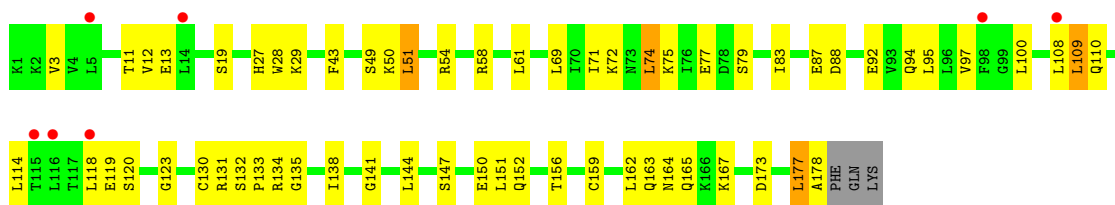


#### • Molecule 1: Envelope glycoprotein gp160

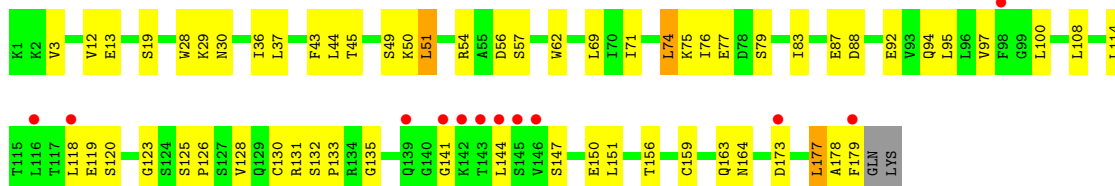


#### • Molecule 2: T-cell surface glycoprotein CD4

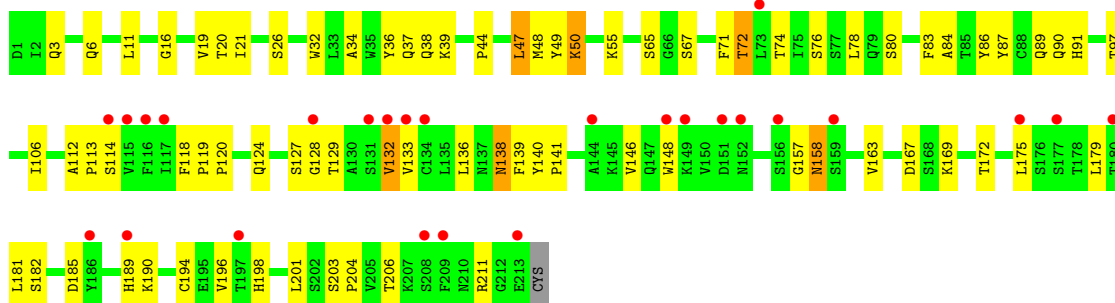




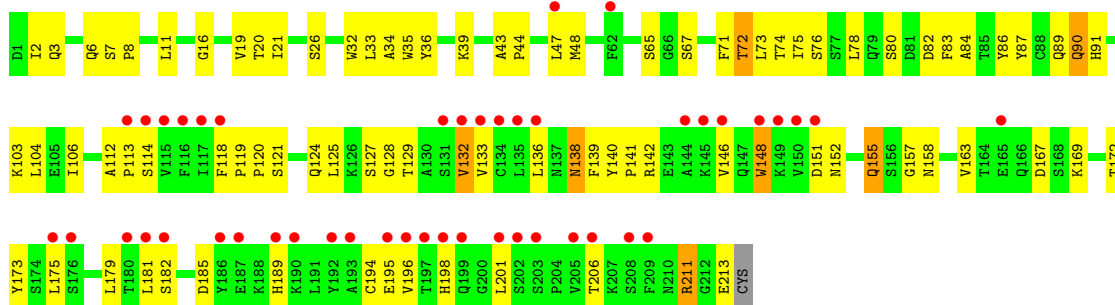
• Molecule 2: T-cell surface glycoprotein CD4



• Molecule 3: anti-HIV-1 antibody 412d light chain

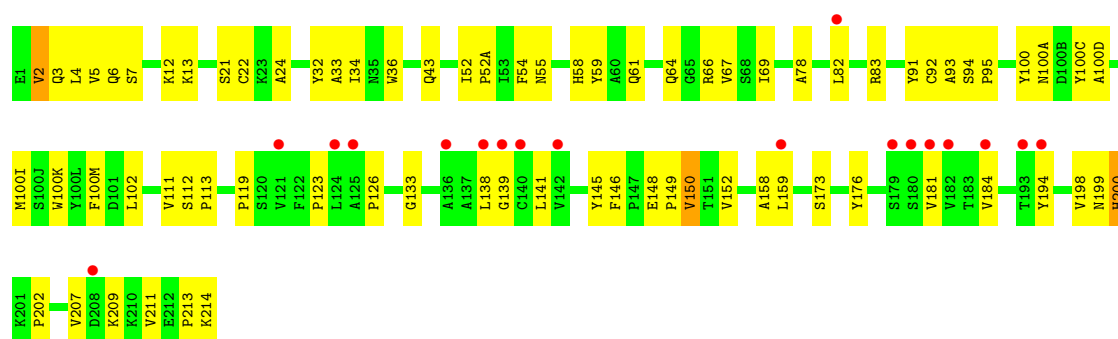


• Molecule 3: anti-HIV-1 antibody 412d light chain

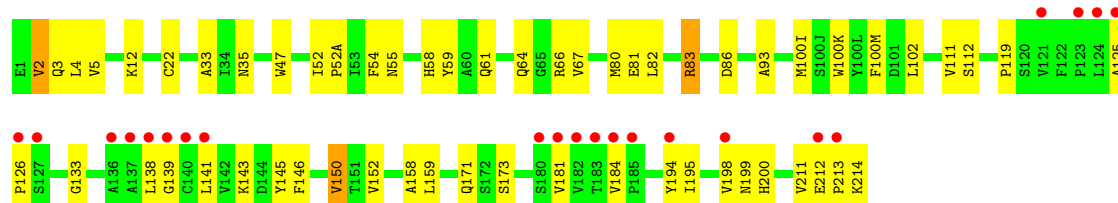
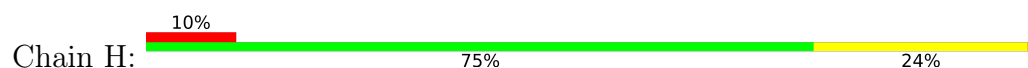


• Molecule 4: anti-HIV-1 antibody 412d heavy chain





• Molecule 4: anti-HIV-1 antibody 412d heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.60Å 53.02Å 225.33Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 49.15 – 3.31	Depositor EDS
% Data completeness (in resolution range)	66.7 (20.00-3.30) 66.4 (49.15-3.31)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX, CNS	Depositor
R, $R_{free}$	0.202 , 0.269 0.205 , 0.204	Depositor DCC
$R_{free}$ test set	1280 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.1	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 104.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.28	0/2546	0.47	0/3446
1	E	0.28	0/2493	0.46	0/3376
2	B	0.25	0/1402	0.44	0/1891
2	F	0.25	0/1414	0.45	0/1907
3	C	0.24	0/1677	0.41	0/2273
3	G	0.25	0/1677	0.42	0/2273
4	D	0.25	0/1757	0.43	0/2393
4	H	0.25	0/1757	0.43	0/2393
All	All	0.26	0/14723	0.44	0/19952

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	2499	0	2443	98	0
1	E	2445	0	2394	86	0
2	B	1383	0	1414	40	0
2	F	1394	0	1423	40	0
3	C	1642	0	1596	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1642	0	1596	66	0
4	D	1746	0	1684	53	0
4	H	1746	0	1684	41	0
5	A	224	0	208	12	0
5	E	210	0	195	6	0
6	A	7	0	3	0	0
6	B	7	0	3	0	0
6	F	7	0	3	0	0
6	H	7	0	3	0	0
7	A	4	0	6	0	0
7	C	8	0	12	0	0
7	D	4	0	6	0	0
7	E	8	0	12	1	0
7	F	4	0	6	0	0
All	All	14987	0	14691	442	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 442 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:B:134:ARG:HH22	2:B:152:GLN:HB3	1.22	1.02
1:A:272:ILE:HG22	1:A:286:VAL:HG22	1.47	0.96
2:F:79:SER:HB3	2:F:97:VAL:HG23	1.52	0.92
4:D:126:PRO:HD2	4:D:213:PRO:HA	1.56	0.87
2:B:79:SER:HB3	2:B:97:VAL:HG23	1.57	0.86

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	315/322 (98%)	275 (87%)	34 (11%)	6 (2%)	9	38
1	E	308/322 (96%)	270 (88%)	32 (10%)	6 (2%)	9	38
2	B	176/181 (97%)	152 (86%)	20 (11%)	4 (2%)	7	33
2	F	177/181 (98%)	152 (86%)	20 (11%)	5 (3%)	5	29
3	C	211/214 (99%)	176 (83%)	30 (14%)	5 (2%)	6	32
3	G	211/214 (99%)	174 (82%)	32 (15%)	5 (2%)	6	32
4	D	227/231 (98%)	185 (82%)	37 (16%)	5 (2%)	7	34
4	H	227/231 (98%)	184 (81%)	38 (17%)	5 (2%)	7	34
All	All	1852/1896 (98%)	1568 (85%)	243 (13%)	41 (2%)	7	34

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	SER
4	D	2	VAL
4	D	150	VAL
2	F	147	SER
4	H	2	VAL

### 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	281/285 (99%)	271 (96%)	10 (4%)	38	68
1	E	276/285 (97%)	260 (94%)	16 (6%)	22	55
2	B	161/164 (98%)	157 (98%)	4 (2%)	50	76
2	F	162/164 (99%)	159 (98%)	3 (2%)	60	80
3	C	188/189 (100%)	183 (97%)	5 (3%)	48	75
3	G	188/189 (100%)	180 (96%)	8 (4%)	32	65
4	D	192/192 (100%)	190 (99%)	2 (1%)	78	87
4	H	192/192 (100%)	189 (98%)	3 (2%)	65	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1640/1660 (99%)	1589 (97%)	51 (3%)	43 72

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	243	SER
1	E	334	SER
3	G	213	GLU
1	E	270	ILE
1	E	352	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	189	HIS
1	E	229	ASN
3	G	137	ASN
4	D	61	GLN
1	E	249	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TYS	D	100	4	15,16,17	1.15	2 (13%)	18,22,24	0.66	0
4	TYS	D	100(C)	4	15,16,17	1.20	2 (13%)	18,22,24	0.53	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TYS	H	100	4	15,16,17	1.16	2 (13%)	18,22,24	0.65	0
4	TYS	H	100(C)	4	15,16,17	1.20	2 (13%)	18,22,24	0.53	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	TYS	D	100	4	-	0/9/11/13	0/1/1/1
4	TYS	D	100(C)	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100	4	-	0/9/11/13	0/1/1/1
4	TYS	H	100(C)	4	-	0/9/11/13	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	100(C)	TYS	OH-CZ	-2.71	1.38	1.42
4	H	100(C)	TYS	OH-CZ	-2.68	1.38	1.42
4	H	100(C)	TYS	CA-C	2.49	1.53	1.50
4	D	100(C)	TYS	CA-C	2.47	1.53	1.50
4	D	100	TYS	OH-CZ	-2.47	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	100	TYS	1	0
4	D	100(C)	TYS	2	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

42 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	MLA	A	3	-	0,6,6	0.00	-	0,7,7	0.00	-
5	NAG	A	734	1	14,14,15	0.52	0	17,19,21	0.71	0
5	NAG	A	741	1	14,14,15	0.60	0	17,19,21	1.41	2 (11%)
5	NAG	A	762	1	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
5	NAG	A	776	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
5	NAG	A	789	1	14,14,15	0.52	0	17,19,21	0.87	1 (5%)
5	NAG	A	795	1	14,14,15	0.55	0	17,19,21	0.61	0
7	EDO	A	8	-	3,3,3	0.47	0	2,2,2	0.32	0
5	NAG	A	801	1	14,14,15	0.51	0	17,19,21	0.66	0
5	NAG	A	832	1	14,14,15	0.50	0	17,19,21	0.99	1 (5%)
5	NAG	A	856	1	14,14,15	0.48	0	17,19,21	0.79	0
5	NAG	A	862	1	14,14,15	0.68	0	17,19,21	1.54	3 (17%)
5	NAG	A	886	1	14,14,15	0.47	0	17,19,21	1.19	2 (11%)
5	NAG	A	894	1	14,14,15	0.42	0	17,19,21	1.12	1 (5%)
5	NAG	A	900	1	14,14,15	0.48	0	17,19,21	1.10	2 (11%)
5	NAG	A	913	1	14,14,15	0.49	0	17,19,21	1.14	2 (11%)
5	NAG	A	948	1	14,14,15	0.53	0	17,19,21	0.60	0
5	NAG	A	963	1	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
6	MLA	B	186	-	0,6,6	0.00	-	0,7,7	0.00	-
7	EDO	C	215	-	3,3,3	0.47	0	2,2,2	0.28	0
7	EDO	C	216	-	3,3,3	0.48	0	2,2,2	0.31	0
7	EDO	D	215	-	3,3,3	0.50	0	2,2,2	0.14	0
7	EDO	E	10	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	E	7	-	3,3,3	0.46	0	2,2,2	0.38	0
5	NAG	E	734	1	14,14,15	0.52	0	17,19,21	0.72	1 (5%)
5	NAG	E	741	1	14,14,15	0.49	0	17,19,21	0.69	0
5	NAG	E	762	1	14,14,15	0.47	0	17,19,21	1.02	1 (5%)
5	NAG	E	776	1	14,14,15	0.48	0	17,19,21	1.54	1 (5%)
5	NAG	E	789	1	14,14,15	0.49	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	795	1	14,14,15	0.52	0	17,19,21	0.77	0
5	NAG	E	801	1	14,14,15	0.49	0	17,19,21	1.25	2 (11%)
5	NAG	E	832	1	14,14,15	0.57	0	17,19,21	0.74	0
5	NAG	E	856	1	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
5	NAG	E	862	1	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
5	NAG	E	886	1	14,14,15	0.55	0	17,19,21	0.94	0
5	NAG	E	894	1	14,14,15	0.54	0	17,19,21	1.34	2 (11%)
5	NAG	E	913	1	14,14,15	0.51	0	17,19,21	1.10	1 (5%)
5	NAG	E	948	1	14,14,15	0.50	0	17,19,21	0.76	0
5	NAG	E	963	1	14,14,15	0.58	0	17,19,21	1.35	3 (17%)
6	MLA	F	186	-	0,6,6	0.00	-	0,7,7	0.00	-
7	EDO	F	187	-	3,3,3	0.48	0	2,2,2	0.25	0
6	MLA	H	215	-	0,6,6	0.00	-	0,7,7	0.00	-

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
6	MLA	A	3	-	-	0/0/4/4	-
5	NAG	A	734	1	-	4/6/23/26	0/1/1/1
5	NAG	A	741	1	-	4/6/23/26	0/1/1/1
5	NAG	A	762	1	-	2/6/23/26	0/1/1/1
5	NAG	A	776	1	-	4/6/23/26	0/1/1/1
5	NAG	A	789	1	-	3/6/23/26	0/1/1/1
5	NAG	A	795	1	-	3/6/23/26	0/1/1/1
7	EDO	A	8	-	-	0/1/1/1	-
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	832	1	-	3/6/23/26	0/1/1/1
5	NAG	A	856	1	-	4/6/23/26	0/1/1/1
5	NAG	A	862	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	886	1	-	3/6/23/26	0/1/1/1
5	NAG	A	894	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	900	1	-	4/6/23/26	0/1/1/1
5	NAG	A	913	1	-	2/6/23/26	0/1/1/1
5	NAG	A	948	1	-	2/6/23/26	0/1/1/1
5	NAG	A	963	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	B	186	-	-	0/0/4/4	-
7	EDO	C	215	-	-	0/1/1/1	-
7	EDO	C	216	-	-	0/1/1/1	-
7	EDO	D	215	-	-	0/1/1/1	-
7	EDO	E	10	-	-	0/1/1/1	-
7	EDO	E	7	-	-	0/1/1/1	-
5	NAG	E	734	1	-	5/6/23/26	0/1/1/1
5	NAG	E	741	1	-	2/6/23/26	0/1/1/1
5	NAG	E	762	1	-	4/6/23/26	0/1/1/1
5	NAG	E	776	1	-	2/6/23/26	0/1/1/1
5	NAG	E	789	1	-	4/6/23/26	0/1/1/1
5	NAG	E	795	1	-	2/6/23/26	0/1/1/1
5	NAG	E	801	1	-	4/6/23/26	0/1/1/1
5	NAG	E	832	1	-	4/6/23/26	0/1/1/1
5	NAG	E	856	1	-	4/6/23/26	0/1/1/1
5	NAG	E	862	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	E	886	1	-	4/6/23/26	0/1/1/1
5	NAG	E	894	1	-	3/6/23/26	0/1/1/1
5	NAG	E	913	1	-	3/6/23/26	0/1/1/1
5	NAG	E	948	1	-	2/6/23/26	0/1/1/1
5	NAG	E	963	1	1/1/5/7	5/6/23/26	0/1/1/1
6	MLA	F	186	-	-	0/0/4/4	-
7	EDO	F	187	-	-	0/1/1/1	-
6	MLA	H	215	-	-	0/0/4/4	-

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	776	NAG	C1-O5-C5	5.19	119.25	112.20
5	A	741	NAG	C1-O5-C5	4.86	118.81	112.20
5	E	801	NAG	C1-O5-C5	4.16	117.86	112.20
5	A	862	NAG	C1-O5-C5	4.15	117.84	112.20
5	E	894	NAG	C1-O5-C5	4.14	117.83	112.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	862	NAG	C1
5	E	862	NAG	C1
5	E	963	NAG	C1
5	A	894	NAG	C1

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	762	NAG	C8-C7-N2-C2
5	A	762	NAG	O7-C7-N2-C2
5	A	963	NAG	C8-C7-N2-C2
5	A	963	NAG	O7-C7-N2-C2
5	E	762	NAG	C8-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	734	NAG	1	0
5	A	776	NAG	2	0
5	A	789	NAG	1	0
5	A	832	NAG	1	0
5	A	862	NAG	2	0
5	A	894	NAG	4	0
5	A	913	NAG	1	0
5	A	963	NAG	1	0
7	E	7	EDO	1	0
5	E	762	NAG	1	0
5	E	789	NAG	3	0
5	E	862	NAG	1	0
5	E	913	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	319/322 (99%)	0.02	5 (1%) 72 70	75, 116, 185, 255	0
1	E	312/322 (96%)	-0.01	3 (0%) 82 82	81, 118, 177, 236	0
2	B	178/181 (98%)	0.09	7 (3%) 39 38	95, 163, 213, 229	0
2	F	179/181 (98%)	0.21	12 (6%) 18 18	96, 163, 213, 228	0
3	C	213/214 (99%)	0.48	26 (12%) 4 4	104, 189, 260, 275	0
3	G	213/214 (99%)	0.87	45 (21%) 1 1	103, 195, 262, 275	0
4	D	229/231 (99%)	0.37	18 (7%) 12 13	92, 157, 259, 288	0
4	H	229/231 (99%)	0.46	22 (9%) 8 9	97, 157, 265, 289	0
All	All	1872/1896 (98%)	0.28	138 (7%) 14 16	75, 147, 250, 289	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	114	SER	10.3
3	G	197	THR	10.1
4	D	125	ALA	7.8
3	C	115	VAL	7.4
2	F	142	LYS	7.4

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

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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	TYS	H	100	16/17	0.95	0.19	129,148,162,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TYS	D	100	16/17	0.95	0.21	130,143,158,167	0
4	TYS	H	100(C)	16/17	0.97	0.19	97,111,132,175	0
4	TYS	D	100(C)	16/17	0.97	0.19	94,108,129,177	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MLA	A	3	7/7	0.29	0.55	175,186,200,209	0
5	NAG	E	856	14/15	0.37	0.45	242,258,275,275	0
5	NAG	A	894	14/15	0.51	0.83	222,258,266,268	0
6	MLA	H	215	7/7	0.52	0.34	181,191,199,201	0
5	NAG	A	900	14/15	0.53	1.38	261,310,326,329	0
5	NAG	A	856	14/15	0.55	0.56	215,243,260,271	0
6	MLA	F	186	7/7	0.56	0.28	180,189,200,207	0
5	NAG	A	963	14/15	0.56	0.76	249,284,309,310	0
5	NAG	E	963	14/15	0.58	0.45	257,278,307,314	0
5	NAG	E	862	14/15	0.61	1.10	208,248,258,260	0
5	NAG	E	894	14/15	0.68	0.65	242,252,258,260	0
7	EDO	F	187	4/4	0.70	0.50	127,128,135,140	0
5	NAG	A	862	14/15	0.70	0.67	214,228,244,250	0
6	MLA	B	186	7/7	0.72	0.34	177,181,190,190	0
5	NAG	E	913	14/15	0.74	0.26	226,244,266,268	0
7	EDO	C	216	4/4	0.76	0.45	148,156,166,167	0
5	NAG	A	913	14/15	0.79	0.25	164,196,225,227	0
7	EDO	E	10	4/4	0.86	0.18	130,139,140,143	0
5	NAG	E	741	14/15	0.88	0.40	192,220,234,236	0
5	NAG	E	832	14/15	0.88	0.24	138,157,187,188	0
7	EDO	C	215	4/4	0.88	0.33	122,127,130,130	0
5	NAG	A	776	14/15	0.88	0.17	137,161,180,185	0
5	NAG	A	741	14/15	0.88	0.30	194,213,222,225	0
5	NAG	A	789	14/15	0.89	0.14	132,155,165,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	734	14/15	0.89	0.20	200,219,224,226	0
5	NAG	E	801	14/15	0.89	0.24	127,177,189,190	0
5	NAG	E	776	14/15	0.90	0.16	128,140,175,175	0
7	EDO	E	7	4/4	0.90	0.25	127,135,139,146	0
7	EDO	A	8	4/4	0.90	0.31	153,153,154,156	0
5	NAG	A	801	14/15	0.90	0.21	134,181,187,191	0
5	NAG	E	886	14/15	0.91	0.24	139,152,191,202	0
5	NAG	A	832	14/15	0.91	0.24	145,167,199,205	0
5	NAG	E	948	14/15	0.91	0.20	116,153,161,163	0
5	NAG	A	734	14/15	0.91	0.17	192,222,231,236	0
5	NAG	A	886	14/15	0.92	0.17	131,151,182,189	0
5	NAG	A	948	14/15	0.92	0.20	124,141,149,156	0
5	NAG	E	795	14/15	0.93	0.18	119,138,146,153	0
5	NAG	E	789	14/15	0.93	0.14	151,182,197,203	0
7	EDO	D	215	4/4	0.93	0.16	100,106,111,111	0
5	NAG	E	762	14/15	0.94	0.26	88,103,115,119	0
5	NAG	A	762	14/15	0.95	0.25	73,97,118,127	0
5	NAG	A	795	14/15	0.96	0.17	89,122,133,145	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.