



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:56 AM GMT

PDB ID : 2C10
Title : THE STRUCTURE OF A TRUNCATED, SOLUBLE VERSION OF SEMIC
ARBAZIDE-SENSITIVEAMINE OXIDASE
Authors : Jakobsson, E.; Kleywegt, G.J.
Deposited on : 2005-09-09
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

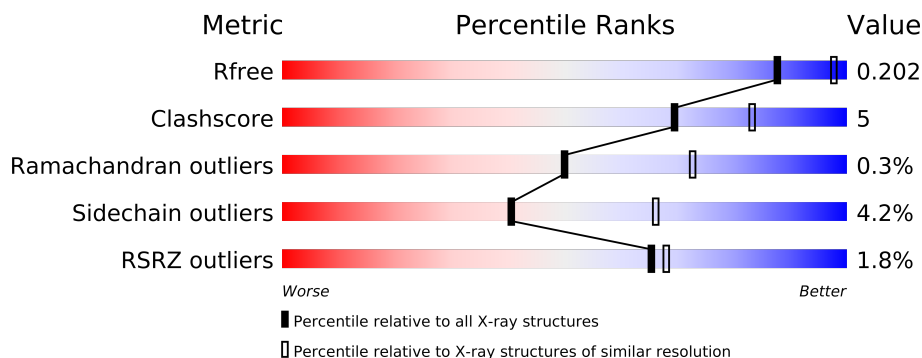
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	735	
1	B	735	
1	C	735	
1	D	735	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	1768	-	X
5	NAG	B	1768	-	X
5	NAG	C	1768	-	X
5	NAG	D	1768	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	D	1774	-	X
8	CL	B	1778	-	X
8	CL	D	1779	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 23470 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	1
			5563	3571	960	1011	21			
1	B	709	Total	C	N	O	S	0	0	1
			5587	3587	965	1014	21			
1	C	706	Total	C	N	O	S	0	0	1
			5563	3571	960	1011	21			
1	D	709	Total	C	N	O	S	0	0	1
			5587	3587	965	1014	21			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		
3	C	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

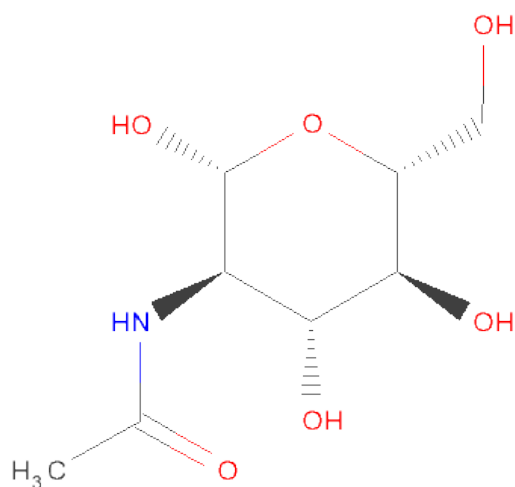
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
6	A	2	Total 2	Ca 2	0	0
6	D	2	Total 2	Ca 2	0	0
6	C	2	Total 2	Ca 2	0	0

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Cu 1	0	0
7	A	1	Total 1	Cu 1	0	0
7	D	1	Total 1	Cu 1	0	0
7	C	1	Total 1	Cu 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total 2	Cl 2	0	0
8	A	2	Total 2	Cl 2	0	0
8	D	2	Total 2	Cl 2	0	0
8	C	2	Total 2	Cl 2	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	5	Total 60	C 34	N 2	O 24	0	0
9	D	5	Total 60	C 34	N 2	O 24	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 11 is water.

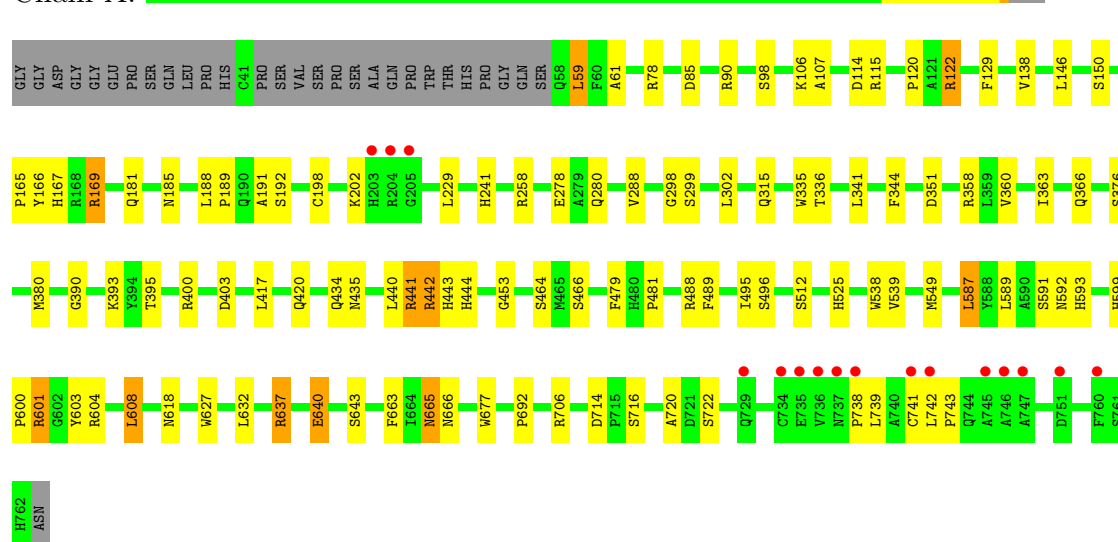
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	141	Total	O	0	0
			141	141		
11	B	139	Total	O	0	0
			139	139		
11	C	141	Total	O	0	0
			141	141		
11	D	142	Total	O	0	0
			142	142		

3 Residue-property plots

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

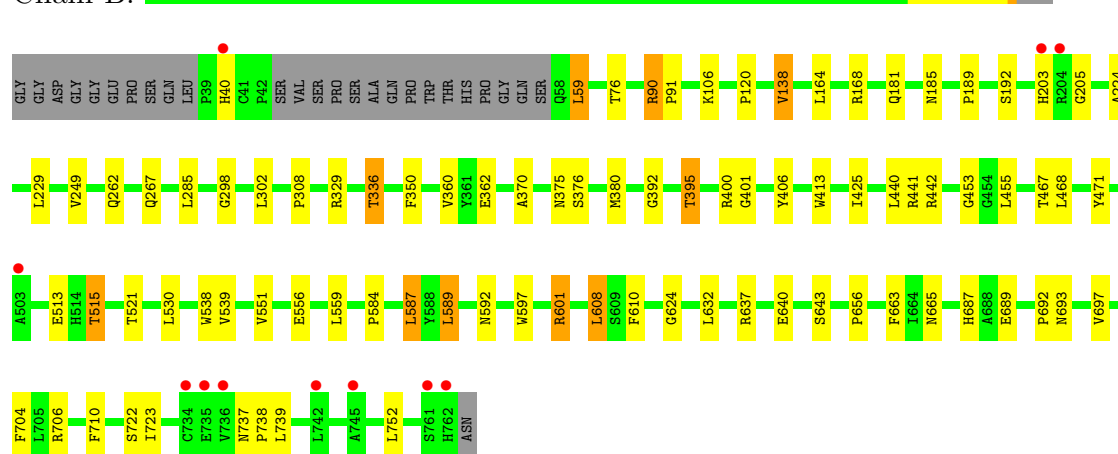
• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain A:



• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

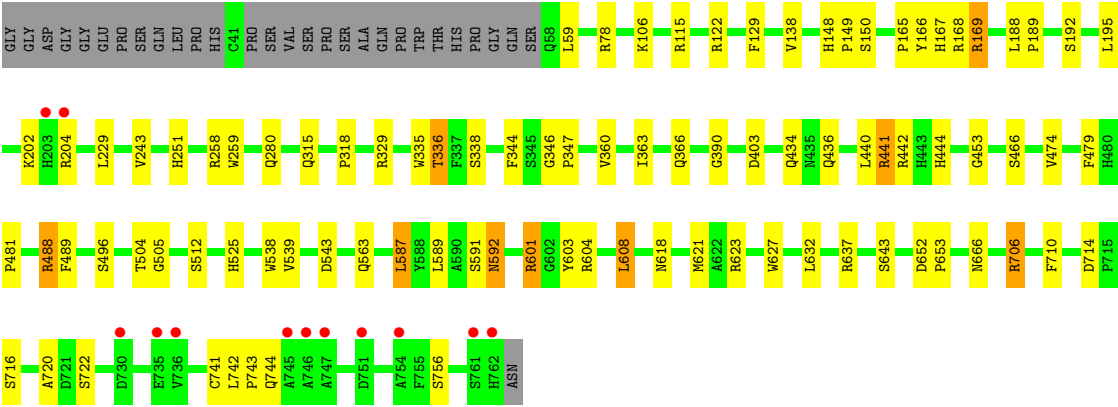
Chain B:



• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

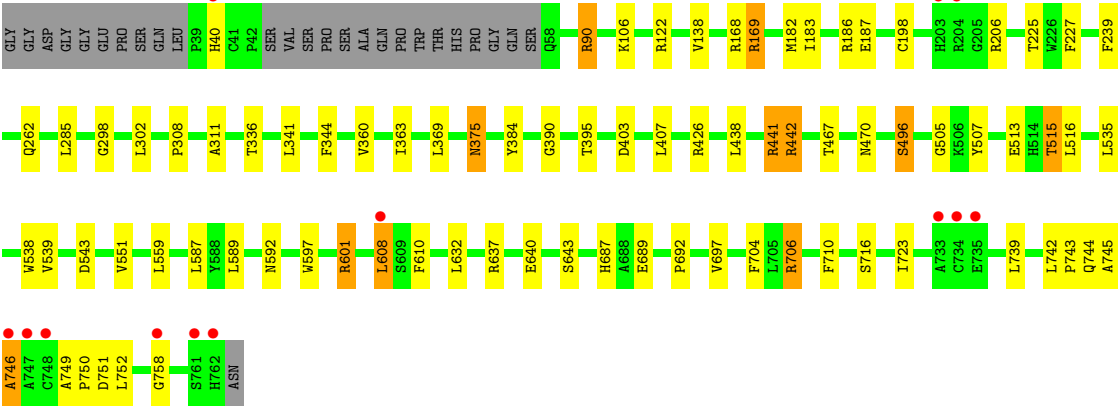
Chain C:





● Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	130.24Å 130.24Å 221.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.50) 98.2 (19.97-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.252 0.200 , 0.202	Depositor DCC
R_{free} test set	6243 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 9.6	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 126403 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23470	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, CL, CA, NDG, TPQ, FUL, CU, 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	0.52	0/5724	0.64	1/7804 (0.0%)
1	B	0.51	0/5751	0.62	1/7842 (0.0%)
1	C	0.51	0/5724	0.62	1/7804 (0.0%)
1	D	0.51	0/5751	0.63	0/7842
All	All	0.51	0/22950	0.63	3/31292 (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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LEU	CA-CB-CG	5.25	127.38	115.30
1	B	589	LEU	CA-CB-CG	5.05	126.93	115.30
1	C	592	ASN	N-CA-CB	-5.00	101.60	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	198	CYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5563	0	5311	69	0
1	B	5587	0	5333	49	0
1	C	5563	0	5311	49	0
1	D	5587	0	5332	57	0
2	A	39	0	34	0	0
2	B	39	0	34	1	0
2	C	39	0	34	0	0
3	A	38	0	34	0	0
3	C	38	0	34	1	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
5	A	14	0	13	1	0
5	B	42	0	39	1	0
5	C	14	0	13	0	0
5	D	42	0	39	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	B	60	0	52	2	0
9	D	60	0	52	0	0
10	D	50	0	43	0	0
11	A	141	0	0	9	0
11	B	139	0	0	4	0
11	C	141	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	142	0	0	5	0
All	All	23470	0	21808	209	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 209 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:360:VAL:HG11	1:D:363:ILE:HG13	1.38	1.04
1:A:360:VAL:HG11	1:A:363:ILE:HG13	1.56	0.85
1:D:426:ARG:HE	1:D:758:GLY:HA3	1.49	0.78
1:A:538:TRP:CZ3	1:A:592:ASN:HB2	2.19	0.77
1:A:488:ARG:HH12	1:A:608:LEU:CD1	1.98	0.77

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	702/735 (96%)	671 (96%)	30 (4%)	1 (0%)	59	81
1	B	704/735 (96%)	675 (96%)	27 (4%)	2 (0%)	50	73
1	C	702/735 (96%)	668 (95%)	32 (5%)	2 (0%)	50	73
1	D	704/735 (96%)	675 (96%)	26 (4%)	3 (0%)	43	66
All	All	2812/2940 (96%)	2689 (96%)	115 (4%)	8 (0%)	50	73

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	ALA
1	C	744	GLN
1	B	59	LEU
1	C	204	ARG

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Mol	Chain	Res	Type
1	B	205	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	585/609 (96%)	555 (95%)	30 (5%)	33	57
1	B	588/609 (97%)	568 (97%)	20 (3%)	49	75
1	C	585/609 (96%)	555 (95%)	30 (5%)	33	57
1	D	588/609 (97%)	569 (97%)	19 (3%)	51	77
All	All	2346/2436 (96%)	2247 (96%)	99 (4%)	40	66

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	640	GLU
1	C	150	SER
1	D	515	THR
1	B	693	ASN
1	C	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	666	ASN
1	B	40	HIS
1	C	185	ASN
1	A	563	GLN
1	B	618	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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$
1	TPQ	A	471	1	14,14,15	5.98	4 (28%)	17,19,21	1.24	2 (11%)
1	TPQ	B	471	1	14,14,15	5.88	4 (28%)	17,19,21	1.17	2 (11%)
1	TPQ	C	471	1	14,14,15	5.83	4 (28%)	17,19,21	1.19	2 (11%)
1	TPQ	D	471	1	14,14,15	5.81	4 (28%)	17,19,21	1.32	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
1	TPQ	A	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	B	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	C	471	1	-	0/4/22/24	0/1/1/1
1	TPQ	D	471	1	-	0/4/22/24	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	O-C	21.22	1.26	1.11
1	B	471	TPQ	O-C	20.75	1.25	1.11
1	C	471	TPQ	O-C	20.57	1.25	1.11
1	D	471	TPQ	O-C	20.44	1.25	1.11
1	D	471	TPQ	O5-C5	4.47	1.37	1.24

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	471	TPQ	C6-C5-C4	2.51	121.59	117.44
1	A	471	TPQ	C6-C5-C4	2.41	121.43	117.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	C6-C1-C2	2.41	120.92	118.24
1	D	471	TPQ	CA-CB-C1	2.35	119.17	114.41
1	C	471	TPQ	C6-C1-C2	2.33	120.83	118.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

37 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	$\# Z > 2$
2	NAG	A	1762	1,2	12,14,15	0.79	0	15,19,21	1.20	2 (13%)
2	NAG	A	1763	2	12,14,15	0.77	0	15,19,21	1.11	1 (6%)
3	NDG	A	1764	1,3	12,14,15	0.84	1 (8%)	15,19,21	1.48	2 (13%)
3	NAG	A	1765	3	12,14,15	0.59	0	15,19,21	1.76	1 (6%)
3	FUL	A	1766	3	9,10,11	0.85	0	10,14,16	0.99	0
4	NAG	A	1767	1,4	12,14,15	0.65	0	15,19,21	1.40	3 (20%)
2	BMA	A	1769	2	10,11,12	0.67	0	11,15,17	0.82	1 (9%)
4	NAG	A	1770	4	12,14,15	0.67	0	15,19,21	0.98	0
2	NAG	B	1762	1,2	12,14,15	0.75	1 (8%)	15,19,21	1.23	2 (13%)
2	NAG	B	1763	2	12,14,15	0.62	0	15,19,21	1.04	1 (6%)
9	NDG	B	1764	1,9	12,14,15	0.64	0	15,19,21	1.40	2 (13%)
9	NAG	B	1765	9	12,14,15	0.66	0	15,19,21	0.85	0
9	FUL	B	1766	9	9,10,11	0.91	0	10,14,16	0.90	0
4	NAG	B	1767	1,4	12,14,15	0.69	0	15,19,21	0.92	1 (6%)
2	BMA	B	1769	2	10,11,12	0.73	0	11,15,17	1.71	2 (18%)
4	NAG	B	1771	4	12,14,15	0.53	0	15,19,21	1.19	1 (6%)
9	BMA	B	1772	9	10,11,12	0.78	0	11,15,17	1.67	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	B	1774	9	10,11,12	0.68	0	11,15,17	0.64	0
2	NAG	C	1762	1,2	12,14,15	0.67	0	15,19,21	1.32	3 (20%)
2	NAG	C	1763	2	12,14,15	0.61	0	15,19,21	0.90	0
3	NDG	C	1764	1,3	12,14,15	0.66	0	15,19,21	1.50	3 (20%)
3	NAG	C	1765	3	12,14,15	0.67	0	15,19,21	2.02	3 (20%)
3	FUL	C	1766	3	9,10,11	0.91	0	10,14,16	1.15	1 (10%)
4	NAG	C	1767	1,4	12,14,15	0.58	0	15,19,21	1.51	2 (13%)
2	BMA	C	1769	2	10,11,12	0.76	0	11,15,17	1.03	1 (9%)
4	NAG	C	1770	4	12,14,15	0.60	0	15,19,21	0.93	0
10	NAG	D	1762	1,10	12,14,15	0.63	0	15,19,21	1.47	2 (13%)
10	NAG	D	1763	10	12,14,15	0.63	0	15,19,21	2.00	5 (33%)
9	NDG	D	1764	1,9	12,14,15	0.67	0	15,19,21	1.27	2 (13%)
9	NAG	D	1765	9	12,14,15	0.47	0	15,19,21	1.63	4 (26%)
9	FUL	D	1766	9	9,10,11	0.83	0	10,14,16	1.50	2 (20%)
4	NAG	D	1767	1,4	12,14,15	0.60	0	15,19,21	0.93	1 (6%)
10	BMA	D	1769	10	10,11,12	0.63	0	11,15,17	1.08	1 (9%)
4	NAG	D	1771	4	12,14,15	0.53	0	15,19,21	1.04	1 (6%)
9	BMA	D	1772	9	10,11,12	0.83	0	11,15,17	1.87	3 (27%)
10	MAN	D	1773	10	10,11,12	0.63	0	11,15,17	1.54	2 (18%)
9	MAN	D	1775	9	10,11,12	0.53	0	11,15,17	1.91	3 (27%)

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
2	NAG	A	1762	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1763	2	-	0/6/23/26	0/1/1/1
3	NDG	A	1764	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1765	3	-	0/6/23/26	0/1/1/1
3	FUL	A	1766	3	-	0/0/17/20	0/1/1/1
4	NAG	A	1767	1,4	-	0/6/23/26	0/1/1/1
2	BMA	A	1769	2	-	0/2/19/22	0/1/1/1
4	NAG	A	1770	4	-	0/6/23/26	0/1/1/1
2	NAG	B	1762	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1763	2	-	0/6/23/26	0/1/1/1
9	NDG	B	1764	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	1765	9	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUL	B	1766	9	-	0/0/17/20	0/1/1/1
4	NAG	B	1767	1,4	-	0/6/23/26	0/1/1/1
2	BMA	B	1769	2	-	0/2/19/22	0/1/1/1
4	NAG	B	1771	4	-	0/6/23/26	0/1/1/1
9	BMA	B	1772	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1774	9	-	0/2/19/22	0/1/1/1
2	NAG	C	1762	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1763	2	-	0/6/23/26	0/1/1/1
3	NDG	C	1764	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1765	3	-	0/6/23/26	0/1/1/1
3	FUL	C	1766	3	-	0/0/17/20	0/1/1/1
4	NAG	C	1767	1,4	-	0/6/23/26	0/1/1/1
2	BMA	C	1769	2	-	0/2/19/22	0/1/1/1
4	NAG	C	1770	4	-	0/6/23/26	0/1/1/1
10	NAG	D	1762	1,10	-	0/6/23/26	0/1/1/1
10	NAG	D	1763	10	-	0/6/23/26	0/1/1/1
9	NDG	D	1764	1,9	-	0/6/23/26	0/1/1/1
9	NAG	D	1765	9	-	0/6/23/26	0/1/1/1
9	FUL	D	1766	9	-	0/0/17/20	0/1/1/1
4	NAG	D	1767	1,4	-	0/6/23/26	0/1/1/1
10	BMA	D	1769	10	-	0/2/19/22	0/1/1/1
4	NAG	D	1771	4	-	0/6/23/26	0/1/1/1
9	BMA	D	1772	9	-	0/2/19/22	0/1/1/1
10	MAN	D	1773	10	-	0/2/19/22	0/1/1/1
9	MAN	D	1775	9	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1764	NDG	O-C5	-2.51	1.40	1.45
2	B	1762	NAG	O5-C5	-2.09	1.41	1.45

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1765	NAG	O5-C5-C6	5.83	113.10	106.98
3	C	1765	NAG	O5-C5-C6	5.58	112.83	106.98
9	D	1772	BMA	C4-C3-C2	4.68	116.78	110.50
2	B	1769	BMA	O5-C5-C6	4.66	111.87	106.98
10	D	1763	NAG	O5-C5-C4	4.40	116.24	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 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	1768	1	12,14,15	0.53	0	15,19,21	1.25	1 (6%)
5	NAG	B	1768	1	12,14,15	0.48	0	15,19,21	0.92	1 (6%)
5	NAG	B	1770	1	12,14,15	0.52	0	15,19,21	2.09	6 (40%)
5	NAG	B	1773	-	12,14,15	0.69	0	15,19,21	1.54	3 (20%)
5	NAG	C	1768	1	12,14,15	0.60	0	15,19,21	1.04	1 (6%)
5	NAG	D	1768	1	12,14,15	0.63	0	15,19,21	1.30	3 (20%)
5	NAG	D	1770	1	12,14,15	0.75	0	15,19,21	1.43	4 (26%)
5	NAG	D	1774	-	12,14,15	0.66	0	15,19,21	1.50	3 (20%)

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	1768	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1768	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1770	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1773	-	-	0/6/23/26	0/1/1/1
5	NAG	C	1768	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1768	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1770	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1774	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1770	NAG	O5-C5-C4	4.60	116.49	110.65
5	A	1768	NAG	O5-C5-C6	3.99	111.17	106.98
5	B	1773	NAG	C2-N2-C7	3.90	129.64	123.09
5	B	1770	NAG	C3-C4-C5	3.67	116.75	110.20
5	D	1774	NAG	C2-N2-C7	3.25	128.54	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	706/735 (96%)	-0.18	16 (2%) 57 60	26, 34, 64, 88	0
1	B	709/735 (96%)	-0.18	11 (1%) 68 71	24, 34, 67, 99	0
1	C	706/735 (96%)	-0.18	12 (1%) 67 69	25, 35, 64, 84	0
1	D	709/735 (96%)	-0.16	13 (1%) 65 68	24, 34, 68, 101	0
All	All	2830/2940 (96%)	-0.17	52 (1%) 65 68	24, 34, 67, 101	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	762	HIS	11.6
1	C	762	HIS	8.0
1	A	203	HIS	6.8
1	C	203	HIS	5.9
1	D	761	SER	5.7

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. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	TPQ	B	471	14/15	0.20	4.04	39,47,49,50	0
1	TPQ	A	471	14/15	0.20	4.02	40,48,51,52	0
1	TPQ	C	471	14/15	0.20	3.98	38,46,49,49	0
1	TPQ	D	471	14/15	0.18	3.16	38,46,49,49	0

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
9	FUL	B	1766	10/11	0.24	5.74	53,55,56,57	0
4	NAG	A	1770	14/15	0.42	3.90	77,81,81,82	0
10	MAN	D	1773	11/12	0.22	3.65	89,90,91,91	0
2	NAG	A	1763	14/15	0.19	2.95	59,63,65,69	0
4	NAG	A	1767	14/15	0.20	2.76	58,64,67,73	0
4	NAG	C	1770	14/15	0.34	2.49	76,79,80,81	0
9	FUL	D	1766	10/11	0.20	1.67	52,55,57,58	0
4	NAG	C	1767	14/15	0.16	1.50	58,64,66,72	0
4	NAG	D	1771	14/15	0.27	1.48	74,75,77,77	0
2	NAG	B	1763	14/15	0.18	1.44	62,66,70,75	0
9	NAG	B	1765	14/15	0.18	1.29	54,61,67,68	0
4	NAG	B	1771	14/15	0.27	1.21	71,73,73,74	0
3	FUL	A	1766	10/11	0.16	1.03	50,51,52,52	0
2	NAG	A	1762	14/15	0.14	1.02	43,46,49,55	0
3	FUL	C	1766	10/11	0.17	0.90	47,50,52,53	0
4	NAG	B	1767	14/15	0.16	0.57	58,63,65,68	0
4	NAG	D	1767	14/15	0.17	0.38	59,66,68,71	0
9	MAN	D	1775	11/12	0.28	0.38	79,81,82,82	0
3	NDG	C	1764	14/15	0.13	0.24	42,48,53,58	0
2	NAG	B	1762	14/15	0.13	0.24	39,43,48,55	0
3	NDG	A	1764	14/15	0.13	0.23	39,44,48,53	0
9	NDG	B	1764	14/15	0.14	0.16	39,45,51,54	0
9	MAN	B	1774	11/12	0.27	0.15	78,79,80,81	0
2	NAG	C	1762	14/15	0.14	0.05	43,49,51,55	0
10	NAG	D	1762	14/15	0.13	-0.19	40,44,49,55	0
9	NDG	D	1764	14/15	0.13	-0.24	34,43,52,52	0
2	NAG	C	1763	14/15	0.13	-0.26	59,61,66,70	0
10	NAG	D	1763	14/15	0.14	-0.95	61,64,68,74	0
2	BMA	C	1769	11/12	0.21	-	73,75,75,76	0
9	BMA	B	1772	11/12	0.14	-	69,70,72,75	0
10	BMA	D	1769	11/12	0.16	-	79,82,86,88	0
3	NAG	C	1765	14/15	0.24	-	62,65,69,69	0
2	BMA	A	1769	11/12	0.24	-	72,74,75,75	0
9	BMA	D	1772	11/12	0.14	-	67,70,72,76	0
9	NAG	D	1765	14/15	0.13	-	55,59,62,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	B	1769	11/12	0.19	-	79,82,82,82	0
3	NAG	A	1765	14/15	0.22	-	57,61,62,62	0

6.4 Ligands

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	C	1768	14/15	0.19	7.18	61,66,66,68	0
5	NAG	D	1774	14/15	0.20	4.27	83,86,87,87	0
8	CL	D	1779	1/1	0.17	4.07	16,16,16,16	0
8	CL	B	1778	1/1	0.15	4.02	18,18,18,18	0
5	NAG	A	1768	14/15	0.22	3.77	64,69,70,70	0
5	NAG	D	1768	14/15	0.15	3.10	62,66,69,70	0
5	NAG	B	1768	14/15	0.17	2.71	62,67,70,71	0
7	CU	D	1777	1/1	0.13	1.19	35,35,35,35	0
6	CA	A	1773	1/1	0.12	0.81	40,40,40,40	0
5	NAG	B	1773	14/15	0.18	0.50	77,78,78,79	0
6	CA	C	1773	1/1	0.12	0.46	42,42,42,42	0
7	CU	B	1776	1/1	0.13	0.27	35,35,35,35	0
6	CA	D	1776	1/1	0.12	0.19	25,25,25,25	0
8	CL	C	1774	1/1	0.14	-0.03	15,15,15,15	0
8	CL	A	1774	1/1	0.15	-0.08	19,19,19,19	0
7	CU	A	1772	1/1	0.12	-0.30	33,33,33,33	0
8	CL	C	1775	1/1	0.13	-0.84	24,24,24,24	1
6	CA	B	1777	1/1	0.11	-0.91	31,31,31,31	0
6	CA	A	1771	1/1	0.09	-1.51	29,29,29,29	0
8	CL	A	1775	1/1	0.10	-1.85	24,24,24,24	1
6	CA	D	1778	1/1	0.10	-1.87	29,29,29,29	0
6	CA	C	1771	1/1	0.10	-1.97	28,28,28,28	0
8	CL	B	1779	1/1	0.10	-2.18	18,18,18,18	1
6	CA	B	1775	1/1	0.10	-2.21	27,27,27,27	0
8	CL	D	1780	1/1	0.08	-2.50	21,21,21,21	1
7	CU	C	1772	1/1	0.10	-3.40	36,36,36,36	0
5	NAG	D	1770	14/15	0.17	-	60,65,67,67	0
5	NAG	B	1770	14/15	0.22	-	60,65,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.